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Science Day 2005 Abstracts

K.M. Kline

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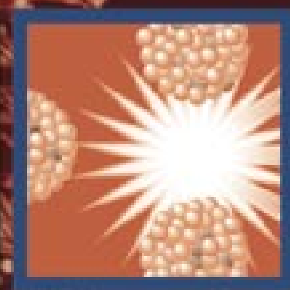
Light & Matter

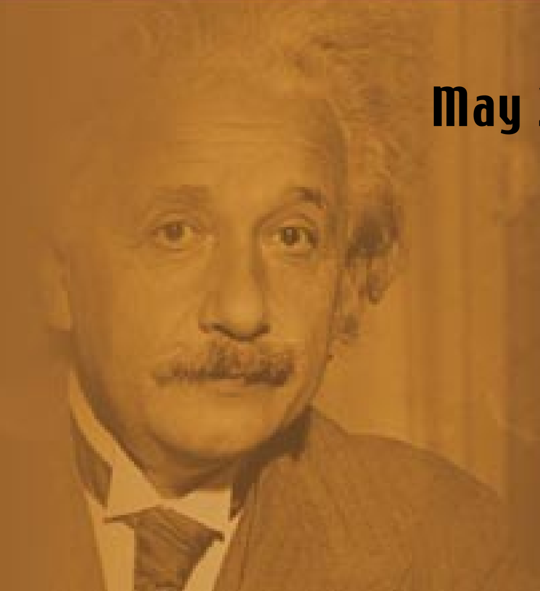

Astrophysics


Theory & Simulations


Biology in Physics


Nuclear Physics

Science Day



May 23, 2005 http://ScienceDay.llnl.gov

LLNL CELEBRATES
The World Year of Physics 2005

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Invited Presentations 01

Abstracts

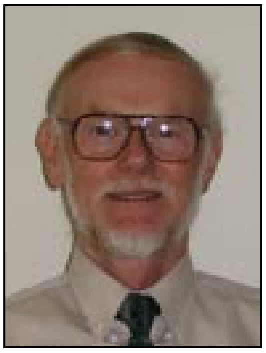
C. Bruce Tarter, Session Chair
Director Emeritus

Session Overview

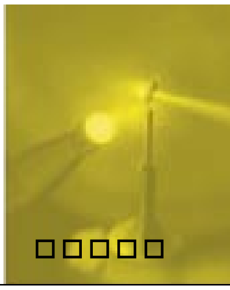
Light & Matter

The interaction of light (especially x rays) and matter have been at the heart of many of the Laboratory's programs since their inception. With the advent of the Laser Program in the '60s, and its subsequent large-scale growth beginning in the early '70s, the coherent and nonlinear optical properties of light have been major research areas. These pursuits directly reflect Einstein's seminal work in what is usually termed his photoelectric effect paper (1905) and his 1917 work on the theory of radiation.

The three talks in this session span a wide range of topics involving light and matter. The first, by Mike Key, will focus on the processes that will occur in experiments at the National Ignition Facility. Nominally, this work will involve the interaction of radiation and matter in very high-temperature (millions of degrees) plasmas. Both the fundamental science involved and its potential role in determining the path to ignition are important physics issues. The second talk, by Claudio Pellegrini, is concerned with very high-intensity light and its applications in coherent sources such as free-electron lasers. Finally, Claire Max will discuss the physics underlying adaptive optics, which has already had wide-ranging applications in fields such as astronomy, biology, and laser fusion.

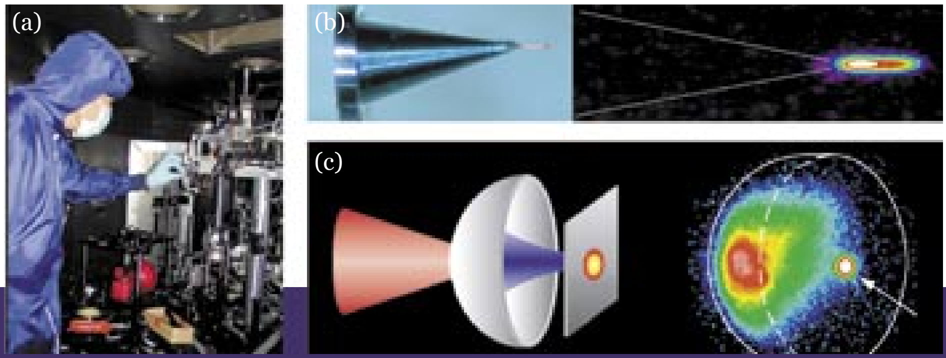


Michael H. Key
Director of Petawatt Science,
National Ignition Facility Programs

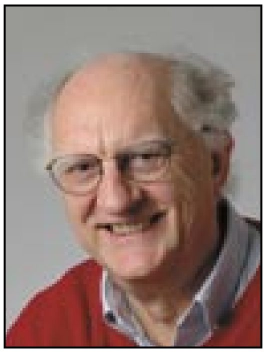


Petawatt: Laser-Based Study of Matter at Extremely High Energy Densities

When people joke that LLNL is an acronym for "Lasers Lasers Nothing (but) Lasers," they wrongly ignore the huge range of science at the Laboratory, but they rightly identify one of the outstanding features of that science. For three decades LLNL has pioneered the extremes of power and energy that can be generated with lasers. The world's first petawatt (PW) (one-thousand-trillion-watt) laser was built at LLNL in 1996, and the first megajoule (one-million-joule) laser, the National Ignition Facility, is now nearing completion in a stadium-sized building that is a landmark feature at the Laboratory. A major motivation for developing such lasers is that they make it possible to create concentrations of energy in small volumes of matter that vastly exceed what can be accomplished in any other way and that mimic conditions in stars and other astrophysical phenomena. Such lasers open the way to precise study of high-energy-density (HED) matter in the Laboratory and present a path to controlled thermonuclear fusion. The President's Office of Science and Technology Policy has made HED science a priority topic. The talk will describe some current experiments in this developing field, highlighting international collaborations and the significant role of graduate students and staff from several U.S. universities. Both the short-term goals of scientific discovery and longer-term possibilities for fusion energy will be outlined. The centenary year of Einstein's seminal work is a fitting opportunity to reflect on his concept of the stimulated emission of light, which provides the basis for all lasers.



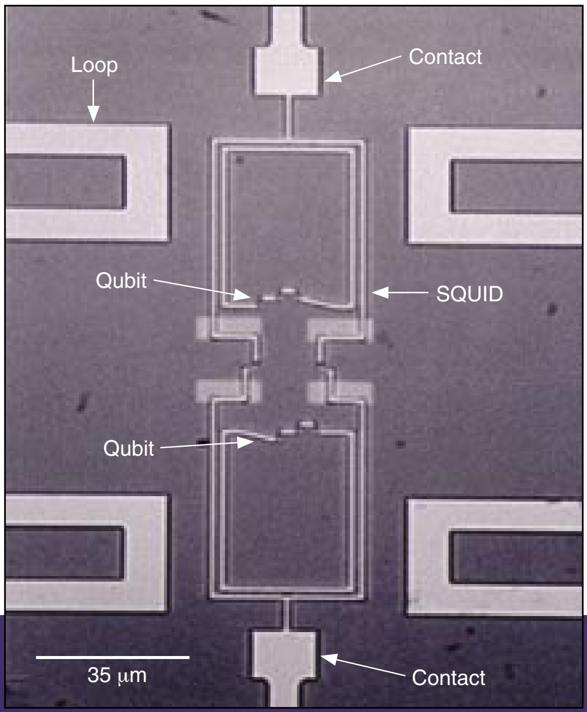
(a) An LLNL scientist adjusts instruments in the vacuum target chamber of the U.K. Vulcan PW laser. (b) *Left*: A hollow cone of aluminum holding a copper wire one-tenth the thickness of a human hair. The Vulcan PW laser was focused into the cone, generating a 100-mega-ampere current of megavolt electrons, which was guided into the wire. *Right*: A characteristic x-ray fluorescence from the copper wire. (c) *Right*: An illustration of the Gekko PW laser in Japan irradiating a 400-micrometer-diameter hemispherical shell and generating a focused beam of megaelectronvolt protons to heat a 100-micrometer-thick aluminum foil. *Left*: An intense spot of thermal x rays (arrow) from the high-energy-density plasma heated by the proton beam.



John Clarke
Professor,
Condensed Matter Physics and Materials Science,
University of California, Berkeley, and
Group Leader, Materials Sciences Division,
Lawrence Berkeley National Laboratory

Superconducting Flux Qubits: Quantum Coherence in a Macroscopic Circuit

The superconducting flux quantum bit (qubit) consists of a superconducting loop interrupted by a weak link known as a Josephson junction. The qubit has two quantum states, consisting of clockwise and anticlockwise supercurrents; its state is measured with a superconducting quantum interference device (SQUID). Microwave spectroscopy reveals that the coherent superposition of the two basis states forms symmetric and antisymmetric wavefunctions, as predicted by quantum mechanics. Manipulation of the states by microwave pulses enables not only observations of Rabi oscillations, Ramsey fringes, and spin echoes, but also measurement of the relaxation and decoherence times. The flux qubit, which is about 100 micrometers in size, thus behaves as a quantum-mechanical, two-state system.



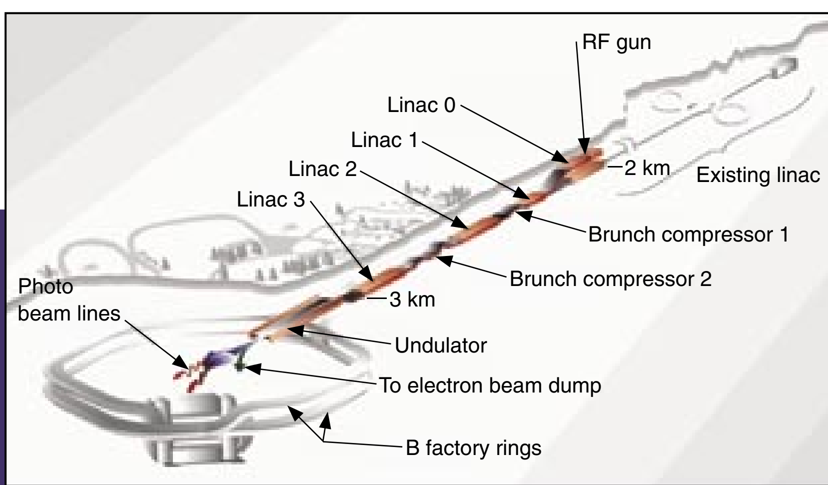
A scanning electron micrograph of a readout superconducting quantum interference device (SQUID) surrounding two flux quantum bits (qubits). The device is fabricated with electron-beam lithography from aluminum films deposited on a silicon chip. The contacts at top and bottom are used to apply current pulses to the SQUID. Currents in the loops provide magnetic flux biases to the qubits and the SQUID.

Claudio Pellegrini
Distinguished Professor of Physics
Department of Physics and Astronomy,
University of California at Los Angeles

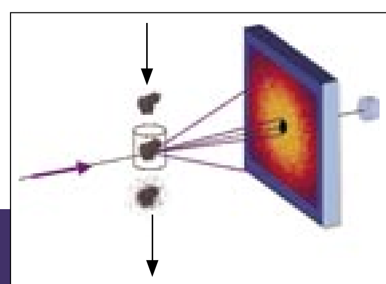
Novel Light Sources: From Synchrotron Radiation to X-Ray Free-Electron Lasers

From the beginning of the seventeenth century—when Galileo first built and used a telescope to explore the Solar System and the stars—our progress in scientific knowledge has often been driven by new developments in optical instruments and light sources, and by our understanding of the nature of light. The discovery of x rays, a little more than a century ago, gave us a tool to explore the structure of living and nonliving matter at the atomic and molecular level.

Einstein's work in 1905, introducing the theory of relativity and the photon as the constituent of light, gave us a new and powerful way to produce light using relativistic electrons beams, and has led to the development of what is today the most brilliant and most widely used source of soft to hard x rays, the storage-ring-based synchrotron radiation source. The next steps in the production of ever-brighter x-ray sources are the Compton backscattering systems, like the Picosecond Laser Electron Interaction for Dynamic Evaluation of Structures (PLEIADES), and the x-ray free-electron lasers. The first x-ray free-electron laser, the Linac Coherent Light Source (LCLS), is now being built by a collaboration of the Argonne National Laboratory, LLNL, Stanford University, the Stanford Linear Accelerator Center, and the University of California, Los Angeles. The LCLS will produce coherent x rays with 10-gigawatt peak power and femtosecond pulse length. The LCLS, due to be completed in a few years, will give scientists the possibility of breaking new ground in the exploration of matter at a length scale of 1 angstrom and a time scale of a few femtoseconds. The many new and exciting experiments that LCLS will enable include the 3-D imaging of a single complex or biological molecule in a single x-ray pulse on a femtosecond time scale, as well as the study of such a molecule's dynamical evolution.



The Linac Coherent Light Source (LCLS), the first x-ray free-electron laser (XFEL), now being built at the Stanford Linear Accelerator Center. When completed, the LCLS will enable the exploration of matter at a length scale of 1 angstrom and a time scale of a few femtoseconds.



With its ultrafast x-ray pulses, an x-ray free-electron laser (XFEL) will allow the imaging of a single molecule hit with a single XFEL pulse. The powerful pulse destroys the molecule, but because of the femtosecond time scale, the image that is computationally reconstructed from the diffracted x rays represents the molecule's intact structure.

William H. Goldstein, Session Chair
Associate Director,
Physics and Advanced Technologies Directorate

Session Overview

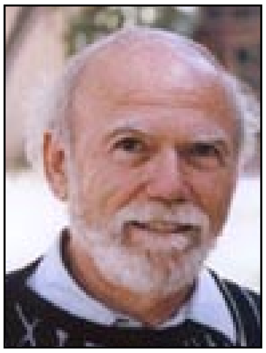
Astrophysics

Astrophysics has been a continuous source of science and scientists to Livermore since its founding. Extreme physical conditions and processes, from nuclear fusion to thermonuclear explosions, are elements common to astrophysical study and Laboratory missions. Remote sensors for nuclear tests and intelligence gathering have been directly based on astronomical instrumentation and techniques, and vice versa.

Einstein provided the scaffold for modern astrophysics and cosmology in 1915, when he published his general theory of relativity, an extension of his special theory of 1905 to treat acceleration (i.e., gravity).

The talks in this session address Einstein's singular impact on our picture of the Universe, and the Laboratory's special connection to astrophysics through two current examples.

The first presentation, by Barry Barrish, director of the Laser Interferometer Gravitational Wave Observatory, will trace the success of the general theory over the last century. In the second talk, John Bradley, director of LLNL's Institute for Geophysics and Planetary Physics, shows that cosmological clues to the origins of the Universe reside in interstellar matter as well as radiation. We are on the verge of capturing a large haul of this material when NASA's Stardust mission returns to Earth; meanwhile, Livermore's extensive suite of state-of-the-art materials-analysis tools is being readied to explore "The Cosmos in a Speck of Dust." Our third talk is by high-energy astrophysicist Bill Craig, who holds joint appointments at LLNL and the Stanford Linear Accelerator Center. He will describe a new NASA-sponsored satellite designed to survey the vast population of black holes that form the cores of galaxies. The mission relies on technological breakthroughs in x-ray optics and detectors that have arisen in the interplay of astrophysics research and LLNL programs in nuclear counterterrorism.



Barry Barish
Director of the Laser Interferometer
Gravitational Wave Observatory, and
Professor of High-Energy Physics
California Institute of Technology

Einstein's Legacy: General Relativity, our Best Description of the Universe

[No abstract available]

Barry C. Barish is the Director of the Laser Interferometer Gravitational Wave Observatory (LIGO) and a professor of high-energy physics at the California Institute of Technology, where he has taught and conducted research since 1963. Barish earned a B.A. in physics in 1957 and a Ph.D. in experimental high-energy physics in 1963 from UC Berkeley.

At Caltech, Barish helped develop a new high-energy physics program that utilized the frontier particle accelerators. Among his noteworthy experiments were those at Fermilab using high-energy neutrinos to reveal the quark substructure of the nucleon. These experiments were among the first to observe the weak neutral current, a linchpin in the Electro-Weak Unification Theory. Barish served as co-chair of the subpanel of the High Energy Physics Advisory Panel that developed a long-range plan for U.S. high-energy physics. He has served as chair of the Commission of Particles and Fields of the International Union of Pure and Applied Physics. Among other activities, he is presently involved in an experiment at the Soudan Underground Mine in Minnesota to further study neutrino properties.

John Bradley
Director
Institute for Geophysics and Planetary Physics

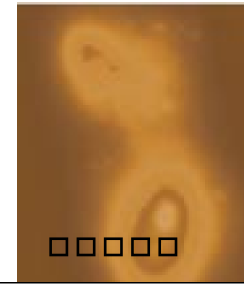
The Cosmos in a Speck of Dust

Dust is a major constituent of the Universe, manifesting itself as obscuring clouds, lanes, globules, and distinctive formations like the famous Horsehead nebula. However, dust has been described as somewhat of an embarrassment in cosmology—we do not believe that it was an important constituent of the early Universe, yet theories rely on clouds of dust cooling and collapsing to form stars, stellar systems, and planetary bodies, some of which provide substrates for the origins and evolution of life.

In interstellar space, dust occurs as submicrometer-sized grains and, although contributing only about one percent of the mass of interstellar space, is almost entirely responsible for the extinction of starlight in the visible region of the spectrum. Trace quantities of ancient (4.5- to 5.5-billion-year-old) interstellar dust are preserved in primitive meteorites and interplanetary dust particles. Interstellar dust was first detected by the Ulysses and Galileo spacecraft.

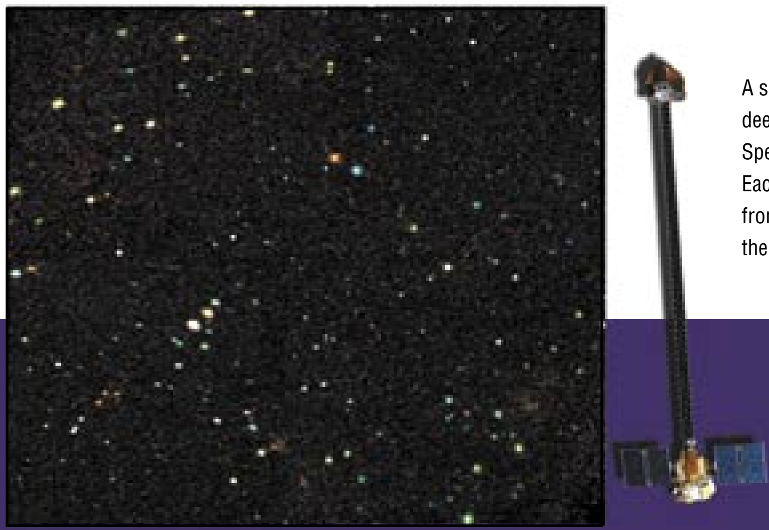
In January 2006, the Stardust mission will return to Earth samples of "fresh" interstellar dust entering the Solar System from the direction of the constellation Scorpio. State-of-the-art electron- and ion-beam instruments, as well as synchrotron facilities, are being employed to probe the elemental and isotopic compositions, as well as the optical properties, of interstellar dust at close to atomic-scale resolution. These studies are providing thrilling insight into the interaction of radiation with solids, the dynamics of supernova explosions, the chemical evolution of the Galaxy, nuclear physics, and the synthesis of organic molecules in interstellar molecular clouds.

William Craig
Advanced Detector Group Leader,
Physics and Advanced Technologies Directorate, and
Staff Scientist,
Kavli Institute for Particle Astrophysics and Cosmoloty Stanford University



Finding Black Holes with the Nuclear Spectroscopic Telescope Array

Over the last five years, astronomers have discovered a previously unknown population of black holes. These ultramassive objects, now known to reside in the cores of most galaxies, can emit copious amounts of hard x rays due to the accretion of matter. At lower photon energies, that emission is often absorbed, by dust and other material in the volume around the black hole. The luminosity of this accretion is quite significant, and may be on par with that of the optical radiation emitted by all the stars in the Universe. Observing this obscured population of black holes has been difficult because of the limited sensitivity of space-borne observatories sensitive to high-energy x-ray radiation. We are now preparing to develop a space-borne mission that enables observations with hundreds of times more sensitivity than the current state of the art. This mission, the Nuclear Spectroscopic Telescope Array (NuSTAR), will use technological breakthroughs in x-ray optics and detectors to image high-energy x rays for the first deep survey of these obscured black holes. As a primary part of its three-year mission, NuSTAR will conduct a census of black holes in selected fields and characterize the black hole population. This talk will cover the evolution of our understanding of the importance of black holes as well as describe the NuSTAR mission and instruments.



A simulation of the results expected from the deep-space survey to be performed by the Nuclear Spectroscopic Telescope Array (NuSTAR) mission. Each bright object is a black hole accreting material from its surroundings. The inset is an illustration of the NuSTAR observatory.

Dona L. Crawford, Session Chair
Associate Director,
Computation Directorate

Session Overview

Theory & Simulations

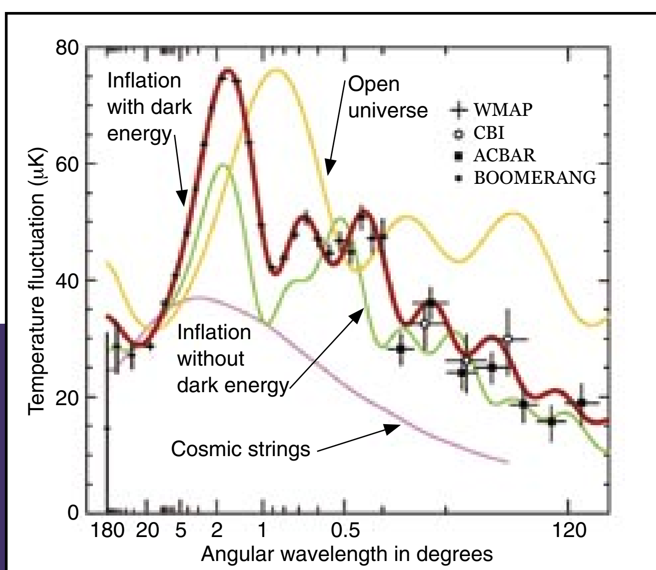
LLNL pushes the frontiers of high-performance computing to help understand materials under extreme temperatures and pressures. In this session, three exceptional researchers examine computational simulation as a tool for modeling and visualizing the physical principles described by Einstein. Specifically, they focus on the challenges inherent in simulating first-principles physics and dislocation dynamics in the modern era.

The first talk in this session, by Giulia Galli, explores the realm of quantum mechanics applied to materials of interest to designers, engineers, and biologists, among others. The crux of these calculations lies in the treatment of the electrons, which, as Einstein anticipated in his photoelectric effects paper of 1905, exhibit both particle and wavelike behaviors. In the second talk, Tomas Diaz de la Rubia will explain how the relatively simple rules of interacting matter can give rise to self-organizing behavior and improved material properties when applied to complex systems. Such research extends Einstein's work on Brownian motion, which relates atomic interaction to observable molecular properties. The final presentation, by Alan Guth, caps the progression away from the micro scale to the grand scale of cosmology. Guth's inflation theory improves the quality of predictions about matter and energy distributions in modern cosmology. The framework for his innovative ideas is supplied by Einstein's theory of general relativity.

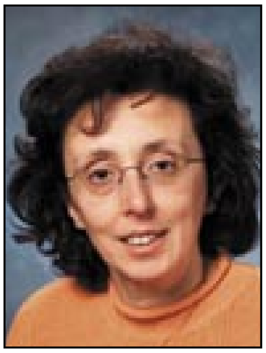
Alan H. Guth
Victor F. Weisskopf Professor of Physics,
Department of Physics,
Massachusetts Institute of Technology

Cosmic Inflation and the Accelerating Universe

This talk will describe the basics of inflationary cosmology, which modifies the "hot" Big Bang theory to offer possible explanations for a number of features of the Universe. In particular, inflation can explain the uniformity of the Universe, the value of its mass density, and the properties of the faint ripples that are now being observed in cosmic background radiation. The cosmic inflation theory even offers a possible explanation for the origin of essentially all matter in the Universe. The recently discovered acceleration of cosmic expansion has radically altered our picture of the Universe, but has also helped to confirm the basic predictions of inflation. When the mass density needed to drive this acceleration is added to the previously known contributions, the result is exactly the value predicted by inflation for the total mass density of the Universe.



A comparison of the latest measurements of the ripples in cosmic microwave background radiation made with several theoretical models, including inflation. The horizontal axis shows the angular wavelength of the fluctuations as seen on the sky, with the shorter wavelengths to the right. The vertical axis shows the strength of the fluctuations of the temperature of the radiation, in microkelvin (μK). The data comes from the Wilkinson Microwave Anisotropy Probe (WMAP) satellite experiment, and from three ground-based experiments: Cosmic Background Imager (CBI), Arcminute Cosmology Bolometer Array Receiver (ACBAR), and Balloon Observations of Millimetric Extragalactic Radiation and Geophysics (BOOMERANG). The red theoretical curve shows the predictions of the simplest inflationary models, including the effects of the dark energy that drives acceleration of the cosmic expansion. This theory is clearly an excellent fit to the data. For comparison, other theoretical curves show the predictions of inflation without dark energy, the prediction for fluctuations generated by the production of objects called cosmic strings, and the predictions for an open Universe, with a mass density of one-quarter of that predicted by inflation.

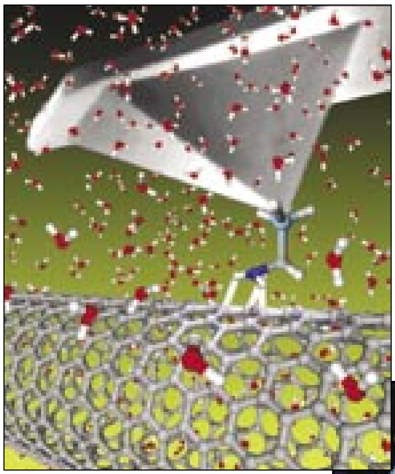


Giulia A. Galli
Quantum Simulations Group Leader,
Physics and Advanced Technologies Directorate

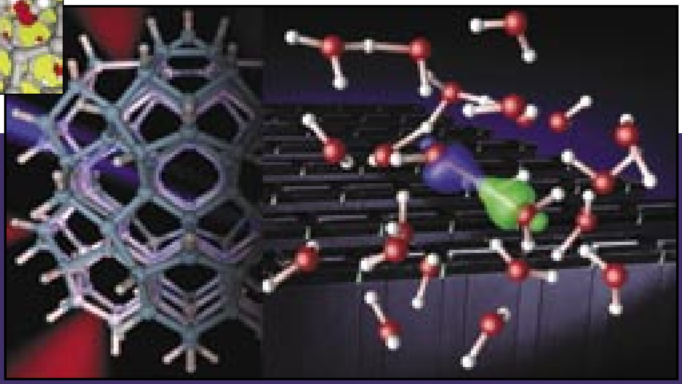
From Empirical Computer Models to Predictive, Ab Initio Simulations

In the past 30 years, the use of scientific computing has become pervasive in all disciplines. The collection and interpretation of most experimental data are carried out using computers; and physical models in computable form, with various degrees of complexity and sophistication, are utilized in all fields. However, using computer simulation in the full prediction of physical and chemical phenomena based on the basic laws of nature is a revolution still in the making. Formidable theoretical and computational challenges must first be overcome.

This talk will illustrate the progress and successes obtained in recent years in predicting fundamental properties of materials in condensed phases and at the nanoscale, using ab initio quantum simulations. The talk will also discuss open issues related to the validation of the approximate, first-principles theories used in large-scale simulations, and the resulting complex interplay between computation and experiment. The focus will be on examples of materials and phenomena at the interface of traditional disciplines—in particular nanomaterials with organic–inorganic interfaces and liquids under extreme conditions. Finally, the talk will briefly cover how computer simulations traditionally used in condensed matter and physical chemistry are being adapted for biochemistry and biology.



Quantum simulations use only the laws of quantum mechanics to predict the behavior of molecules and condensed matter from the fundamental interactions of electrons and ions. These simulations are ideal tools for examining the atomic and electronic structure of materials. The Figure shows a quantum simulation of the attachment of a molecule to a carbon nanotube in the presence of water.



Predictive calculations of nanostructures, such as the slicon quantum dots (left), and condensed systems, such as compressed water (right), are enabled by advances in quantum simulations, combined with LLNL's high-performance computers.

Tomás Diaz de la Rubia
Associate Director,
Chemistry and Materials Science Directorate

From Planetary Interiors to the Mechanics of Materials: Computational Chemistry and Materials Science at the Terascale

New theoretical and computational developments, coupled with the increasing availability of ever more powerful, massively parallel computers, have made large-scale simulation an essential tool in the arsenal of the materials scientist and the chemist. When combined with well-designed laboratory experiments, simulation enables the scientist to perform previously impractical or impossible experiments and to explore the manner in which complexity in material behavior arises from a set of relatively simple underlying physical laws.

This talk discusses two recent examples of scientific discovery achieved with large-scale simulation. The first concerns recent investigations of the structure of water under the extremely high pressures and temperatures typical of giant planetary interiors. Simulations and experimentation both indicate the existence of a nonmolecular superionic phase of water, in which oxygen atoms are frozen but hydrogen atoms are melted. Superionic water may actually be common in our Solar System. The second example involves the development of a new three-dimensional dislocation dynamics code, ParaDis, which enables simulations of materials deformation at a scale as small as tens of micrometers. These simulations show that unexpected topological defects arise in the microstructure of body-centered-cubic (bcc) metals as a metal deforms. These defects, called multinodes, are the result of many-body dislocation collisions and had never before been considered in the theory of dislocations. Multinodes have been shown to govern the strength of a bcc metal—and are believed to be fundamentally responsible for the irreversibility of plastic deformation in such metals. The talk will conclude with a brief discussion of future challenges.

Elbert W. Branscomb, Session Chair
Associate Director,
Biociences Directorate

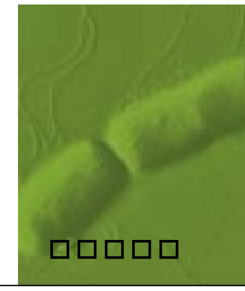
Session Overview

Physics in Biology

Albert Einstein, who is most popularly famous for the theory of relativity, published his paper on the special theory of relativity in 1905. But at that time, he was at least as preoccupied by questions of statistical physics—and the quantal nature of energy—as he was by the physics of space–time. His interest in the former subject was driven largely by a desire to comprehend and demonstrate the particulate or atomistic nature of both matter and energy and the connection this had to their statistical and thermodynamic properties. This work led to a flurry of papers—most notably two papers in 1905 on Brownian motion and on the photoelectric effect—and a paper in 1906 on the heat capacity of solids.

In reference to his own work on Brownian motion, Einstein remarked, "My major aim in this was to find facts which would guarantee as much as possible the existence of atoms of definite, finite size." In reference to his work on the photoelectric effect (for which he was awarded the Nobel Prize in 1921): "This way of looking at the problem showed in a drastic and direct way that a type of immediate reality has to be ascribed to Planck's quanta, that radiation must, therefore, possess a kind of molecular structure in energy."

The importance of Einstein's contributions in this general area is hard to overstate. Max Born wrote: "In my opinion [Einstein] would be one of the greatest theoretical physicists of all times even if he had not written a single line on relativity." Indeed, Einstein's publications in statistical and quantum physics played a key role in making the atomic theory of matter and the corpuscular nature of energy real and palpable. By doing so, his work stimulated and directed the early development of quantum theory and, through that the achievement, the development of a fundamental understanding of chemistry, molecular structure, physical chemistry, thermodynamics, and a great deal more. On this foundation rests all science that depends on understanding the behavior of energy and matter at the molecular scale, including the modern science of biology. In this important sense, the contribution of Einstein's work to biology is simply immense. However, the direct



connections between physics and the everyday work of biology have been, and are still, almost paradoxically slight.

The rather incredible flowering that both physics and biology have experienced in parallel in the last 100 years seems most remarkable not only for the shear magnitude of advances achieved, but for two other features: how humble they both were as sciences in 1905, and how little the progress of biology has so far owed directly to physics or physicists.

In 1905, the atomic theory of matter was still in question—and biology was also in at least as primitive a state. The particulate nature of inheritance, Mendelism, was only just broaching the gates of accepted belief. The role chromosomes had in transmitting "character" or in shaping development was still highly unclear. Essentially, nothing of life's molecular basis—the "central dogma" drama of DNA, genes, RNA, transcription, translation, proteins, and the rest—was known or even guessed. The comparative immensities of what we now understand about life's devices have all been achieved since then. But notably, between then and now, biologists have almost never been driven to learn physics or employ physicists. Once given the keys to chemistry and the life of molecules by the early quantum physicists, biologists have had little further need of physics. But in fact, biology has come only a little way and is only just now really getting started. As never before in the history of biology, "the times they are a-changin." The revenge of physics is surely upon us.

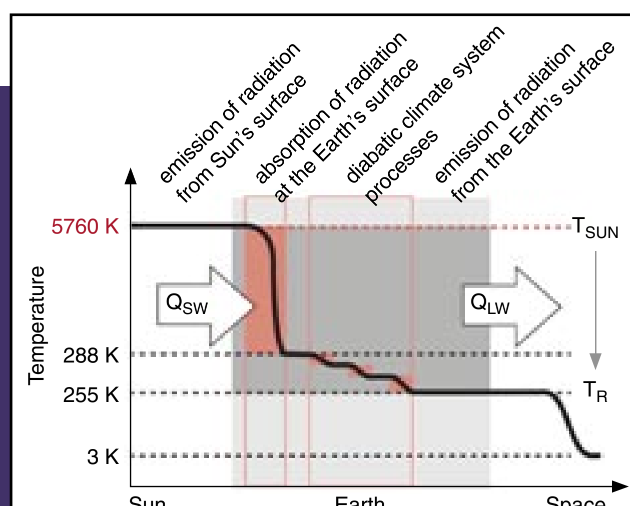
In this session, we will hear talks from three scientists who are leading research in different directions, all of which illustrate this point. Dr. Steven Block will discuss the use of optical tweezers to study biological motors. Dr. George Oster will speak on protein motion, propulsion, and pattern formation in biological systems. And, finally, Dr. Axel Kleidon will discuss the application of nonequilibrium thermodynamics to understanding life, climate, and the coupling between them. All three of these topics clearly echos the issues that concerned Einstein 100 years ago, and the advances he made in understanding.

Axel Kleidon
Assistant Professor in Earth System Science
University of Maryland

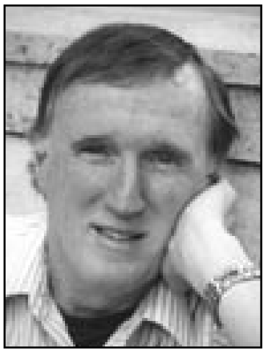
Einstein, Thermodynamics, and Life on Earth

Thermodynamics played a central role in shaping Einstein's thoughts and career. In his own words, thermodynamics "is the only physical theory of universal content that ... will never be overthrown." Einstein's work was seminal in shaping the quantum view of electromagnetic radiation, which extended the range of statistical mechanics and thermodynamics far beyond the ideal gas. On Earth, solar radiation, a flux of highly energetic photons, drives Earth-system processes and photosynthetic activity, which in turn provides the "fuel" for abundant life. The degradation of this energy flux to lower temperatures allows processes on Earth to perform work, dissipate energy, and produce entropy. Entropy production—the degradation of energy into forms less able to perform work—is a general direction for Earth system processes, ranging from the planetary energy balance to the global hydrological cycle and the cycling of carbon by the Earth's biosphere.

This talk will discuss an extension of the concepts of statistical mechanics to non-equilibrium systems—systems that produce entropy in steady state, such as any life form on Earth, as well as the Earth system as a whole. The principle of maximum entropy production (MEP) states that at the macroscopic scale, systems work the hardest, thereby producing entropy at the maximum possible rate allowed by the constraints imposed on the system. One of the unique features of Earth from an MEP perspective is that the amount of absorbed solar radiation, and therefore the rate of planetary entropy production, is not fixed but strongly shaped by the presence of ice and cloud cover. Thus the entropy rate is an emergent property of the climate system. Life, by its inherent diversity, adds many degrees of freedom to the surface-exchange fluxes of energy, water, and carbon and to the emergent climate on Earth. This talk suggests that with this added flexibility, a life-bearing Earth maximizes the planetary rate of entropy production, making life a highly probable and predictable emergent phenomenon of the Earth system. Closing the talk will be a discussion on the relevance of this thermodynamic perspective for the Earth system's response to global change.



Earth-system processes, including life, transform a flux of highly energetic solar photons (QSW), which begin at the solar temperature (TSUN), towards subsequently lower temperatures. This eventually results in the emission of longwave radiation (QLW) to space, which represents a flux of many more photons that are much less energetic. This direction towards lower temperatures allows Earth-system processes to perform work and dissipate energy and results in the production of entropy. Thus, life plays a central role in the magnitude of entropy production of Earth system processes.



George Oster
Professor of Cell and Developmental Biology
and Environmental Science, Policy, and Management,
University of California, Berkeley

Protein Motion, Propulsion, and Pattern Formation

[No abstract available]

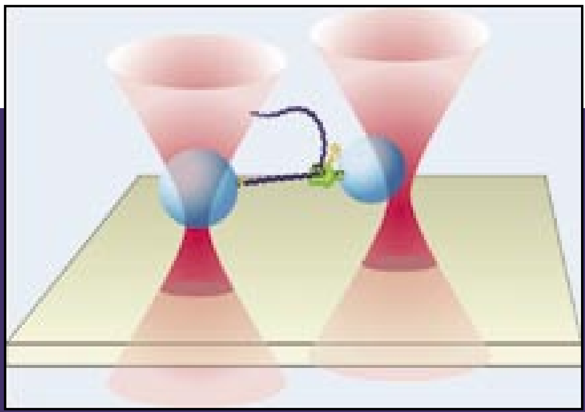
Dr. George Oster is a Professor of Cell and Developmental Biology and of Environmental Science, Policy, and Management at the University of California, Berkeley. His research has involved the construction and testing of theoretical models of molecular, cellular, and developmental processes. He received a B.S. from the Merchant Marine Academy in 1961 and a Ph.D. from Columbia University in 1967. His current projects include investigations into the basic physics and chemistry of protein motors, cell motility and spatial pattern formation in eukaryotic and prokaryotic cells, and membrane protein organization.

Steven M. Block
Professor,
Departments of Applied Physics and Biological Sciences,
Stanford University

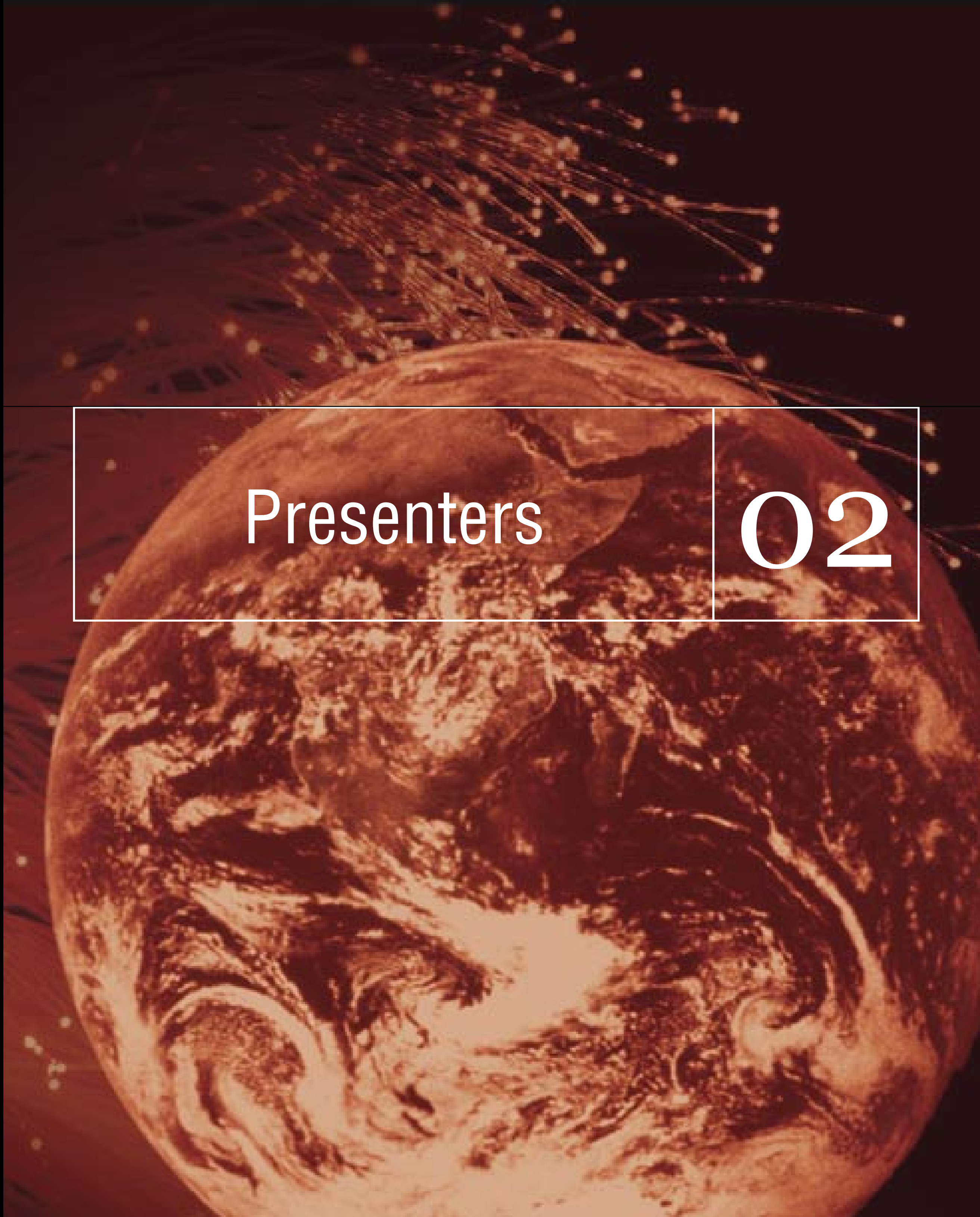
Using Optical Tweezers to Study Biological Motors

"Optical tweezers," also known as optical traps, use radiation pressure produced by laser light to grasp and manipulate tiny dielectric particles, usually in the size range of tens of nanometers up to a few micrometers. With a judicious choice of laser power and wavelength, these particles are manipulated to grasp—in a tweezer-like, nondamaging way—small objects in an aqueous environment, even living specimens, such as individual cells or bacteria. Optical tweezers are extraordinarily versatile and robust, with many potential applications in science and technology, particularly when combined with other useful technologies, such as interferometry, nanometry, and advanced fluorescence methods. (For an annotated bibliography of the optical trapping field, see M.J. Lang & S.M. Block, *Am. J. Phys.* **71**:201–215, 2003.) The greatest utility of optical tweezers thus far has come in the new interdisciplinary area of single-molecule biophysics, where optical traps have been used successfully to study the nanoscale properties of individual biological macromolecules such as proteins and nucleic acids. At this level, fundamental limits imposed by Brownian motion and diffusion play an important role, not only in the measurement process, but in the function of the macromolecules themselves. This talk will cover recent progress in the area of single-molecule biophysics at the current limits of its resolution.

An illustration of the experimental geometry of a high-resolution "dumbbell" assay used to study gene transcription by single molecules of RNA polymerase (not to scale). Two micrometer sized polystyrene beads (blue) are suspended above a microscope coverglass (beige) by infrared laser-based optical traps (red). A DNA molecule, initially 1 micrometer long, is held between the twin beads under variable tension using computer feedback. The bead on the left is directly attached to one end of a DNA template molecule (navy blue). The bead on the right is attached by a streptavidin linkage (yellow) to a single molecule of RNA polymerase (green), which transcribes the DNA into RNA (orange). As transcription proceeds, the DNA is drawn through the polymerase molecule, shortening the end-to-end distance of the dumbbell tether and causing the right bead to move away from the trap center. This motion can be measured with subnanometer precision.



Presenters 02



Presenters

C. Bruce Tarter
Director Emeritus

C. Bruce Tarter was the Director of LLNL from 1994 to 2002, the eighth director to lead the Laboratory since it was founded in 1952. During his tenure as Director, Bruce Tarter led the Laboratory in its mission to ensure national security and apply science and technology to the important problems of our time. He has served as Director Emeritus since 2002. A theoretical physicist by training and experience—he received a bachelor's degree in Physics from MIT and a Ph.D. from Cornell University—he began his career at the Laboratory in 1967. He is a Fellow of the American Physical Society and the American Association for the Advancement of Science, and received the Roosevelts Gold Medal Award for Science in 1998, the National Nuclear Security Administration Gold Medal in 2002, and the Secretary of Energy's Gold Award in 2004.

Claudio Pellegrini
Distinguished Professor of Physics,
University of California, Los Angeles

Claudio Pellegrini received the "Laurea in Fisica" and the "Libera Docenza" from the University of Rome. From 1958 to 1978 he worked at the Frascati National Laboratory, where, in 1976, he was named division director. From 1978 to 1989 he was the Associate Chairman of the National Synchrotron Light Source and Co-chairman of the Center for Accelerator Physics at Brookhaven National Laboratory. In 1989 he joined the faculty of UCLA, where he is now a Distinguished Professor of Physics. He also served as the Chair of the Physics and Astronomy Department from 2001 to 2004.

His research is mostly on high-energy physics colliders, synchrotron radiation sources and free-electron lasers (FELs). In the 1960s, he discovered the head-tail instability and other collective effects limiting the collider's luminosity. Later, he developed the theory of high gain FELs in the self-amplified spontaneous emission regime and used these results to propose and design and an x-ray FEL. In the 1990s, he led his group at UCLA to give the first experimental verifications of this theory, the base of the U.S. x-ray FEL project.

Professor Pellegrini is a Fellow of the American Physical Society. A CERN Fellow in 1985 and a Fulbright Fellow in 1997, he was awarded the International FEL prize in 2000, and the Wilson Prize of the American Physical Society in 2001.

George Oster

Professor of Cell and Developmental Biology and Environmental Science, Policy, and Management, University of California, Berkeley

Dr. George Oster is a Professor of Cell and Developmental Biology and of Environmental Science, Policy, and Management at the University of California, Berkeley. His research has involved the construction and testing of theoretical models of molecular, cellular, and developmental processes. He received a B.S. from the Merchant Marine Academy in 1961 and a Ph.D. from Columbia University in 1967. His current projects include investigations into the basic physics and chemistry of protein motors, cell motility and spatial pattern formation in eukaryotic and prokaryotic cells, and membrane protein organization.

Axel Kleidon

Assistant Professor in Earth System Science, University of Maryland

Axel Kleidon received a highly interdisciplinary education. He received an M.S. in physics at Purdue University in 1994. In 1998, at the Max Planck Institute for Meteorology in Hamburg, Germany, he completed doctoral research on the role of the depth of the vegetation rooting zone in the climate system. As a postdoctoral scientist at Stanford University, he developed an innovative approach to modeling the relationship of the climate with patterns of plant biodiversity—work inspired by his background in physics. Since 2001, he has been an assistant professor at the University of Maryland, in both the Department of Geography and at the Earth System Science Interdisciplinary Center. His research there focuses primarily on understanding the functional role of terrestrial vegetation in the climate system, the mechanisms by which vegetation moderates the effects of global change, and on the controversial Gaia hypothesis, which states that the Earth system is regulated "for and by the biosphere." Over the last few years, he has been increasingly interested in applying, nonequilibrium thermodynamics and the principle of maximum entropy production to Earth system science, a topic on which he has recently co-edited a book (Springer, 2004).

www.earthsystem.org

Michael H. Key
Director of Petawatt Science,
National Ignition Facility Programs

After receiving his B.S. and Ph.D. at Imperial College in London, Mike was appointed to a faculty position at Queens University, Belfast, in 1967, where he developed high-power pulsed lasers and studied laser-produced plasmas and x-ray lasers. When the U.K. established a national laser facility at the Rutherford Appleton Laboratory (RAL) in 1977, he first coordinated its scientific program and later joined its permanent staff. He became Director of the RAL laser department in 1983, and in 1989 he added the role of Professor and Research Group Leader at Oxford University. In 1996, he was recruited to the Inertial Confined Fusion (ICF)/National Ignition Facility (NIF) Program at LLNL, where he was Deputy Scientific Director for ICF/NIF. He is currently Director of Petawatt Science for NIF.

Mike was a German Humboldt Fellow in 1972–3. The U.K. Institute of Physics and the German Physical Society awarded him the Max Born Medal and Prize in 1995 for his international role in developing x-ray lasers and in developing excimer and neodymium glass lasers and their application to high-intensity light–matter interaction. With colleagues, he received the German Max Planck *ForschungsPreis* in 1991 for work on krypton-fluoride lasers and, the Anglo-Japanese Daiwa Foundation Award in 1993 for work on x-ray lasers. He received the Edward Teller Award in 1997 for work in the field of laser fusion, and became a Fellow of the American Physical Society in 1999, in recognition for his work on x-ray backlighting and x-ray lasers. He has authored some 350 papers and given over 100 invited talks.

Alan H. Guth
Victor F. Weisskopf Professor of Physics,
Department of Physics,
Massachusetts Institute of Technology

Alan H. Guth is the Victor F. Weisskopf Professor of Physics and a Margaret MacVicar Faculty Fellow at the Massachusetts Institute of Technology (MIT). Trained in particle theory at MIT, where he obtained a Ph.D. in physics in 1972, he held postdoctoral positions at Princeton, Columbia, Cornell, and the Stanford Linear Accelerator Center (SLAC) before returning to MIT as a faculty member in 1980. His work in cosmology began at Cornell, when Henry Tye persuaded him to study the production of magnetic monopoles in the early Universe. Using standard assumptions, they found that far too many monopoles would be produced. Continuing this work at SLAC, Guth discovered that the magnetic monopole glut could be avoided with a new proposal that he called the inflationary universe. He is a member of the National Academy of Sciences and the American Academy of Arts and Sciences, and has been awarded the Franklin Medal for Physics of the Franklin Institute, the Dirac Prize of the International Center for Theoretical Physics, and the Cosmology Prize of the Peter Gruber Foundation. He is still busy exploring the consequences of cosmic inflation, and has written a popular-level book on that subject, titled *The Inflationary Universe: The Quest for a New Theory of Cosmic Origins*.

William H. Goldstein

Associate Director,
Physics and Advanced Technologies Directorate

William H. Goldstein leads the Physics and Advanced Technologies (PAT) Directorate at LLNL. The Directorate is a diverse research and development organization comprising roughly 300 Ph.D. scientists. Its mission is to provide frontier physics and technology for 21st-century national security missions: stockpile stewardship, homeland security, energy independence, and the exploration and utilization of space.

The PAT Directorate is home to programs in high-pressure physics, condensed-matter physics, plasma physics, nuclear and high-energy physics, radiation detection, optical science, medical technology, fusion energy, and the Livermore branch of the University of California.

Since joining the Laboratory in 1985 (from a post-doctoral position at the Stanford Linear Accelerator Center), Goldstein has been heavily involved in developing the Stockpile Stewardship Program. He served as Program Leader for Physical Data Research, with responsibility for providing equation-of-state, opacity, and nuclear data for nuclear weapon simulations. Before that, he was a Deputy Division Leader in the Physics and Space Technology Directorate, and Computational Physics Group Leader in the Nuclear Test and Experimental Science Directorate.

Bill Goldstein received a B.A. in physics from Swarthmore College in 1977 and a Ph.D. in theoretical physics from Columbia University in 1983. He received the Weapons Recognition of Excellence Award in 1995 for his work on radiative opacity. A member of the American Physical Society, he has authored or co-authored over 70 papers in the fields of elementary particle theory, nuclear physics, atomic physics, x-ray physics, and plasma spectroscopy.

Giulia Galli
Quantum Simulations Group Leader,
Physics and Advanced Technologies Directorate

Giulia Galli is the Quantum Simulations Group Leader in the Physics and Advanced Technologies Directorate. She received a Ph.D. in Physics from the International School for Advanced Studies in Trieste, Italy. After postdoctoral positions at the University of Illinois at Urbana-Champaign and the IBM Research Division in Zurich, she joined the Swiss Institute of Technology in Lausanne, where she was Senior Researcher and then Senior Scientist. In 1998 she came to LLNL as a Staff Scientist and became group leader two years later. In 2000, she received a Department of Energy award of excellence for technical excellence in advanced simulations, and in 2004 received the Science and Technology LLNL Award. She is a fellow of the American Physical Society (APS) and 2005 Chair-Elect of the Division of Computational Physics of the APS. She serves on the executive committee of APS for the California Section, as well as on numerous national and international editorial and advisory boards. Her current research activity is focused on quantum simulations of materials in condensed phases and at the nanoscale, with focus on interdisciplinary problems. She is the author of more than 130 peer-reviewed papers published in international scientific journals.

Tomás Díaz de la Rubia
Associate Director
Chemistry and Materials Science Directorate

As associate director for the Chemistry and Materials Science Directorate (CMS), Tomás Díaz de la Rubia manages more than 520 chemists, chemical engineers, materials scientists, and physicists. The directorate is responsible for multidisciplinary research and technology development in support of the Laboratory's missions in national security, energy and environment, and biotechnology.

Díaz de la Rubia joined the Laboratory in 1989 in a postdoctoral appointment. Subsequently, he served as a term scientist in CMS, a staff physicist, and as the scientific capabilities leader for Computational Materials Science. In 2000, he was appointed deputy division leader for Science and Technology in the Materials Science and Technology Division of CMS. He also held a concurrent position leading a team of CMS scientists who brought expertise to the National Ignition Facility (NIF) project—specifically, solving the potential issue of 3-omega damage on NIF's final optics. In 2001, Díaz de la Rubia became Materials Program leader for NIF Programs in addition to leading the Lasers–

Materials Interaction Investment area in CMS. He earned a B.S., *summa cum laude*, in physics in 1984 and a Ph.D., also in physics, in 1989, both from State University of New York.

The author of more than 130 publications in the areas of computer simulation of physical properties and performance of materials, Díaz de la Rubia is also an active member of the scientific community and has chaired national and international conferences. He is a Fellow of the American Physical Society and is on the board of directors of the Materials Research Society.

Dona L. Crawford

Associate Director,
Computation Directorate

As associate director for Computation at LLNL, Dona Crawford is responsible for the development and deployment of an integrated computing environment for terascale simulations of complex physical phenomena. This environment includes high-performance computers, scientific visualization facilities, high-performance storage systems, network connectivity, multi-resolution data analysis, mathematical models, scalable numerical algorithms, computer applications, and necessary services to enable mission goals and scientific discovery through simulation. She has served on advisory committees for the National Science Foundation, the National Research Council, and the Council on Competitiveness. She is a member of the board of directors of the Civilian Research and Development Foundations, the Institute of Electrical and Electronics Engineers, and the Association for Computing Machinery. Dona is also active in the High-Performance Networking and Computing Conference series, and participates in community-outreach activities to promote math and science.

William Craig

Advanced Detector Group Leader,
Physics and Advanced Technologies Directorate, and
Staff Scientist,
Kavli Institute for Particle Astrophysics and Cosmology,
Stanford University

William Craig graduated from the University of California, Berkeley (B.A, M.S., and Ph.D.) in Physics Sciences. After working as a postdoc at LLNL he spent five years at Columbia University, where he conducted research on supernova remnants and developed instrumentation for high-energy astrophysics. He returned to LLNL in 2000 and developed a platform to fly a balloon-borne hard-x-ray telescope, a program which eventually led to the selection of the space mission known as the Nuclear Spectroscopic Telescope Array (NuSTAR) http://www.nustar.caltech.edu/. He leads the LLNL portion of the NuSTAR instrument development and also serves as NuSTAR project scientist. Craig also is involved in transferring the radiation-detection technology from the astrophysics program to the emerging homeland security mission. Craig also holds an appointment as staff scientist at the Kavli Institute for Particle Astrophysics and Cosmology at Stanford.

John Clarke

Professor, Condensed Matter Physics and Materials Science, University of California, Berkeley, and Group Leader, Materials Sciences Division, Lawrence Berkeley National Laboratory

John Clarke received his degrees from Cambridge University, England: a B.A. in 1964, an M.A. and Ph.D. in 1968, and an Sc.D. in 2003. He came to the University of California, Berkeley as a postdoctoral scholar in 1968; the following year, he became a member of the faculty and a faculty senior scientist at LBNL.

His research has focused on the fundamental science and applications of superconductivity. In particular, he has worked on an ultrasensitive detector of magnetic flux known as the superconducting quantum interference device (SQUID). Currently, in collaboration with colleagues, he is using SQUIDs to obtain magnetic resonance images in a magnetic field four orders of magnitude lower than in conventional scanners. He is also working with colleagues in the UC Berkeley Physics Department and at LBNL to develop SQUIDs for the readout of detectors used to measure the cosmic microwave background. In addition, he is collaborating with a group at LLNL to install a SQUID amplifier in their experimental setup to search for the axion—a candidate for cold dark matter. He is also applying SQUIDs to study quantum coherence in superconducting flux quantum bits.

John Clarke is a fellow of the Royal Society and has received a number of awards for his research, including the Keithley Award of the American Physical Society, the Comstock Prize of the National Academy of Sciences, the Hughes Medal of the Royal Society, and the first Lounasmaa Prize of the Finnish Academy.

Elbert Branscomb

Associate Director,
Biociences Directorate

Elbert received a B.A. in physics from Reed College in Portland, Oregon, in 1957 and a Ph.D. in theoretical physics from Syracuse University in 1964. That year, he joined LLNL as a theoretical physicist, making the transition to biosciences in the late 1960s. He held the position of senior research biologist until being named the founding Director of the Joint Genome Institute in 1996, a position he held until 2000. In November 2000, Elbert was named Chief Scientist, U.S. Department of Energy Genome Program, through which he participated in the formulation of the Genomes-to-Life Initiative. In 2004 he was named associate director of the Biosciences Directorate. Elbert has served on numerous scientific advisory and grant-review panels for the National Institutes of Health and the Department of Energy.

John P. Bradley

Director
Institute for Geophysics and Planetary Physics

John Bradley is the director of the Institute for Geophysics and Planetary Physics. Since 1996, he has also held the position of Adjunct Professor in the School of Materials Science and Engineering at Georgia Institute of Technology. He earned a B.S. in chemistry from the University of Canterbury, Christchurch, New Zealand in 1976 and a Ph.D. in chemistry from Arizona State University in 1982. That year, he conducted postdoctoral research in the Department of Astronomy at the University of Washington in Seattle. He was a Senior Research Scientist with McCrone Associates in Chicago (1983–1992). Prior to joining the Laboratory, Bradley was the Executive Director of MVA Inc., a privately held company that specializes in materials science consulting and research for industry and the federal government. He is a member of the American Association for the Advancement of Science, a Fellow of the Meteoritical Society and the Microbeam Analysis Society.

Steven M. Block

Professor,
Department of Applied Physics and Biological Sciences,
Stanford University

Steve Block is a biophysicist holding a joint appointment in Biological Sciences and Applied Physics at Stanford University. He is also a Senior Fellow of Stanford's Institute for International Studies and a member of JASON. Prior to joining Stanford in 1999, Block held positions at Princeton University (1994–1999), Harvard University (1987–1994), and the Rowland Institute for Science (1987–1994). Trained in both physics and biology, Block graduated from Oxford University (1974), received his doctorate from Caltech (1983), and did postdoctoral work at Stanford (1985–7). He was the recipient of the 1994 Young Investigator Award of the Biophysical Society, and is a

Fellow of the American Academy of Arts and Sciences. He currently serves as President of the Biophysical Society. Block's interdisciplinary research lies at the interface of physics and biology, particularly the study of motor proteins. His laboratory pioneered the use of laser-based optical traps ("optical tweezers") to study the nanoscale motions of single biomolecules. His group was the first to resolve the individual, 8-nm steps taken by kinesin motors moving along microtubules, and the ~5-bp backtracking motions made by RNA polymerase when it proofreads errors in DNA transcription. Biological systems studied in his lab include kinesin, RNA polymerase, exonuclease, and helicase, as well as nucleic acids (DNA and RNA). Block is a proponent of nanoscience and the applications of biology to nanotechnology, but also an outspoken critic of the futurist element of the nanotechnology movement. In the public policy arena, Block has written and spoken extensively about the emerging threat of bioterrorism. He led an influential 1997 study on the impact of genetic engineering on biological warfare, and currently serves on an National Academy of Sciences committee on next-generation biological threats. In what little spare time he has, he plays bluegrass banjo, guitar, and mandolin.

Barry Barish

Director, Laser Interferometer Gravitational Wave Observatory, and Professor, High-Energy Physics, California Institute of Technology

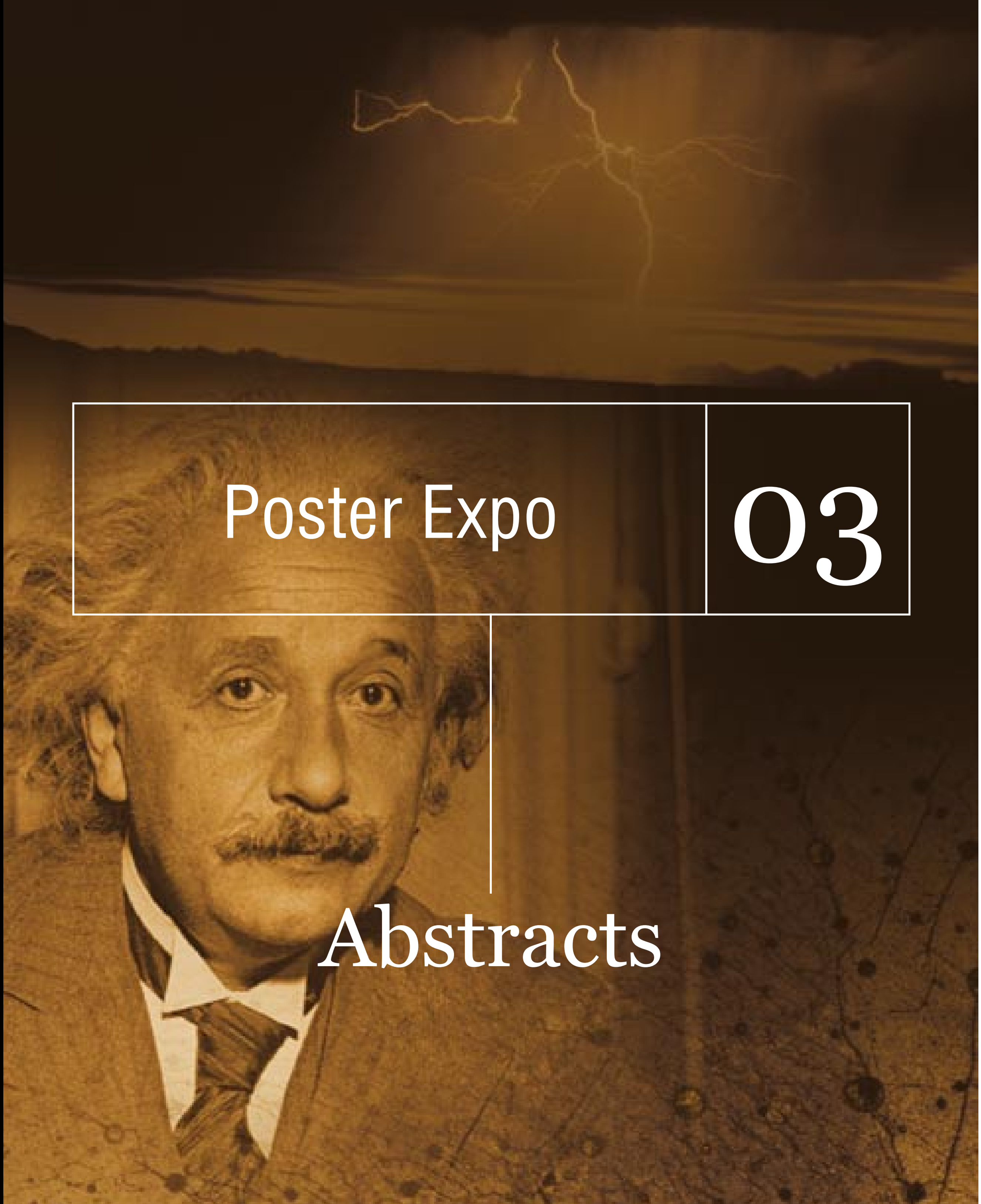
Barry C. Barish is the Director of the Laser Interferometer Gravitational Wave Observatory (LIGO) and a professor of high-energy physics at the California Institute of Technology, where he has taught and conducted research since 1963. Barish earned a B.A. in physics in 1957 and a Ph.D. in experimental high-energy physics in 1963 from UC Berkeley.

At Caltech, Barish helped develop a new high-energy physics program that utilized the frontier particle accelerators. Among his noteworthy experiments were those at Fermilab using high-energy neutrinos to reveal the quark substructure of the nucleon. These experiments were among the first to observe the weak neutral current, a linchpin in the Electro-Weak Unification Theory. Barish served as co-chair of the subpanel of the High Energy Physics Advisory Panel that developed a long-range plan for U.S. high-energy physics. He has served as chair of the Commission of Particles and Fields of the International Union of Pure and Applied Physics. In 2002 he received the Klopsteg Award of the American Association of Physics Teachers and was elected to the National Academy of Sciences. Since being nominated to the National Science Board in October 2002, He has advised the President and Congress on policy issues related to science, engineering, and education. Since 2003, he has served on the special NASA panel that is considering the future of the Hubble Space Telescope and the transition to the James Webb Space Telescope. Bary is also presently involved in an experiment at the Soudan Underground Mine in Minnesota to further study neutrino properties.

George Oster

Professor, Cell and Developmental Biology
and Environmental Science, Policy, and Management,
University of California, Berkeley

Dr. George Oster is a Professor of Cell and Developmental Biology and Environmental Science, Policy, and Management at UC Berkeley. His research has involved the construction and testing of theoretical models of molecular, cellular, and developmental processes. He received a B.S. from the Merchant Marine Academy in 1961 and a Ph.D. from Columbia University in 1967. His current projects include investigations into the basic physics and chemistry of protein motors, cell motility and spatial pattern formation in eukaryotic and prokaryotic cells, and membrane protein organization.



Poster Expo 03

Abstracts

Light & Matter

This research funded by Laboratory Directed Research and Development

The Quantum Nature of Light: Using Highly Charged Uranium to Test Quantum Theory with Unprecedented Accuracy

Peter Beiersdorfer

Modern atomic spectroscopy makes it possible to study, with ultrahigh precision, the discrete energy quanta of light predicted in one of Einstein's 1905 papers. LLNL's electron beam ion trap, called SuperEBIT, produces highly charged ions of any element, including uranium with all electrons removed. SuperEBIT measures the energy of the light quanta given off by these ions to detect energy shifts caused by large relativistic effects associated with the very high velocity at which an electron orbits the nucleus of a highly charged ion. This velocity approaches a significant fraction of the speed of light. Such relativistic effects are another manifestation of one of Einstein's papers from 1905. Super EBIT measurements are precise enough for testing theories that go beyond Einstein: quantum electrodynamics that predicts further energy shifts due to vacuum fluctuations from position–electron pair production and annihilation based on a combination of Einstein's famous $E = mc^2$ concept and the Heisenberg Uncertainty Principle, as well as the interaction of a given electron with its own sea of "bound" photons. Our recent SuperEBIT measurement of U^{89+} (i.e., uranium with only three remaining electrons) is the most accurate in the world for testing quantum theories in the superhigh fields of highly charged ions.

Hot Hohlraums and Albert Einstein

Marilyn Schneider

Visible lasers are converted into x-ray sources inside tiny cylindrical cavities called hohlraums, which means "hollow rooms" in German. The radiation spectrum, or how much energy is present at each wavelength inside the hohlraum, is described by the blackbody formula derived by Max Planck in 1900. This formula assumed that light energy can only occur at certain discrete values, or quanta. In 1905, Albert Einstein explained why light is quantized: light has a dual nature—it is both a wave and a particle.

Hot hohlraums are hotter than other hohlraums because all the available laser energy is put into a smaller container in a shorter time. The laser energy ionizes and evaporates (or ablates) the hohlraum wall material, forming a plasma, which quickly fills the tiny hohlraum and scatters the laser light. The description of the plasma is based on kinetic theory. In 1905, Albert Einstein's paper on kinetic theory and Brownian motion developed the fundamental equations that described the motion of atoms (and later ions) in fluids and plasmas. This poster describes recent experiments on hot hohlraums on the

NIF laser that have led to new understanding of laser–plasma coupling.

Short-Pulse Laser Absorption and Solid-Target Heating at Relativistic Laser Intensities

Ronnie Shepherd

We have embarked on an exciting new program to study the effects of solid matter heated with short-pulse, high-intensity (>10^{18} W/cm^2) laser beams. At these laser intensities, the electric field of the laser is so large that it can accelerate electrons to relativistic velocities. As a result, the pondermotive force begins to alter the density profile, an electrostatic-driven ion shock is predicted to form, the relativistic mass of the electrons increases the penetration depth of the laser, and magnetic fields that can exceed 3 gigagauss are generated inside the target. Furthermore, the oscillatory velocity (v_{os}) asymptotically becomes large compared to thermal velocity (v_{th}), suggesting a significant amount of vacuum heating and relativistic $J \times B$ heating. The poster presents theory and experimental data showing the laser absorption and subsequent target heating resulting from high-intensity, short-pulse generation of relativistic electrons in laser–solid interactions.

Relativistic Plasma Simulations

A. B. Langdon

Short-pulse lasers concentrate as much as a kilojoule of energy down to a picosecond and into a very small area. The very large electromagnetic fields near the focal spot oscillate electrons to nearly the speed of light. As described by the special theory of relativity, the electrons' mass increases at such speeds. The resulting nonlinearity in plasma response to the wave produces a rich variety of light propagation instabilities and accelerates electrons to relativistic energies. The Fast Ignitor concept for inertial confinement fusion exploits some of these properties. "Particle-in-cell" computer models provide a first-principles treatment of the relativistic, nonlinear, and kinetic effects.

Pair Production and Positron Annihilation

Scott Wilks

In this poster, we present recent experimental and theoretical research devoted to creating relativistic pair plasmas. Positrons, the antimatter equivalent of electrons, are identical to electrons in everyway except that positrons have a positive charge. Being antimatter, positrons cannot exist long on Earth as they annihilate after about a billionth of a second when they collide with electrons, i.e. matter. This annihilation is perhaps the most striking

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example of the equivalence of mass and energy because all of the mass of these two particles (an electron and a positron) is turned completely into energy, usually in the form of two gamma rays. Similarly, with enough energy in a small volume of space, one can create electron–positron pairs out of pure energy. Our current research does just this: creating a large number of pairs using ultraintense lasers. In addition, it turns out that the pairs we create are extremely energetic, so energetic that we must use relativity (as described in the first of Einstein's 1905 papers) to describe their motion properly. Astrophysicists think relativistic pair plasmas are present in many compact objects throughout the Universe. We hope to create such plasma in the laboratory for a fraction of a second, in hopes of gaining a better understanding of the cosmos around us.

Electron Speedometer for Solid-Density Plasmas

Gianluca Gregori

Expanding on Einstein's explanation of the photoelectric effect, the theory of scattering of x rays by electrons was formulated in the 1920s by several illustrious physicists (Debye, Compton, Dirac, and Chandrasekhar). They and others realized that the Doppler shift caused by an x ray scattering off an electron could be used to infer the speed and direction of electrons in solid matter (the Compton effect). Today, we are using this effect as a probe of the transient electron velocity distribution, and hence temperature, of solid-density, low-atomic-number plasmas that are prevalent in high-energy-density physics and inertial-confinement, fusion capsules, but cannot be measured through optical or x-ray spectroscopy means. The data are being used to validate various equation-of-state models developed by the statistical plasma physics community. New research has also begun in extending the technique to probe collective electron motion in dense plasmas for which no experimental data exist.

Superconducting Ultrahigh-Energy-Resolution X-Ray, Gamma-Ray, and Neutron Spectrometers

Stephan Friedrich

Superconducting spectrometers operated at temperatures of ~0.1 K offer an order of magnitude improvement in energy resolution over conventional semiconductor Ge and Si(Li) detectors. This greatly increases the sensitivity in a wide area of scientific applications, ranging form high-energy astrophysics to biophysics and material science. The Advanced Detector Group is developing sensors based on the resistive superconducting-to-normal transition, as well as the refrigeration and readout technology to

make detector operation at ~0.1 K user-friendly. This poster presents the current state-of-the-art superconducting detector technology, and illustrate its wide potential with representative high-precision measurements on active metal sites in proteins, novel semiconductors and special nuclear materials.

Hyperspectral Imaging

Charlie Bennet

One of Einstein's most important contributions to physics was the elucidation of the multidimensional nature of space-time. Relativity theory intimately connects the three dimensions of space with the fourth dimension of time. In his later years, Einstein tried heroically to develop a unified theory of physics that brought in extra dimensions. In recent years, string theorists have suggested that there may actually be ten spatial dimensions.

In the field of hyperspectral imaging, the data from imaging spectrometers are represented as having a large number of extra dimensions, with an extra dimension corresponding to each of the different spectral colors observed. Among its various applications, hyperspectral imaging has proven effective for detecting and identifying art forgeries and has been used in the medical arena for health diagnostics.

Past, Present, and Future of Relativistic Optical Technology at LLNL

Chris Barty

For nearly two decades, LLNL has been at the forefront of high-peak-power, short-pulse laser technology development. This technology makes it is possible to enter a new regime of laser–matter interactions in which the focused laser field strength is sufficient to accelerate free electrons to relativistic velocities on a single half-cycle of the laser oscillation. This new regime, which has been called the “relativistic optical” regime, occurs at focused laser intensities of approximately 10^{18} W/cm^2 and can be easily reached with modern terawatt and petawatt laser technology. In the relativistic optical regime, the extreme velocities and strong magnetic fields in the laser focus lead to a new and fundamentally different “longitudinal” coupling of the laser light to matter. With relativistic intensities, it is possible to produce intense, forwardly directed beams of tens of keV to multiple-MeV electrons, which may in turn be used to create unique sources of short-duration, high-energy, x-rays and collimated beams of energetic protons and ions. This poster reviews the past, present and future development of relativistic optical technology at LLNL. The history ranges from the production of some of the first terawatt-peak-power laser pulses on a single benchtop,

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to demonstration of the first petawatt pulses on the Nova laser system, to the development of new technologies that may eventually enable exawatt-peak-power pulse production on NIF. In all phases, LLNL has played a leadership role in the development of advanced short-pulse laser architectures and advanced laser component technology.

Watching Crystals Melt in Real Time with Ultrafast X-Ray Vision

Fred Hartemann

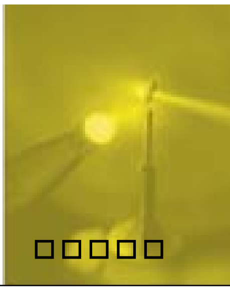
LLNL is developing new ultrafast x-ray and gamma-ray sources to resolve fundamental unanswered solid-state physics questions, including the dynamics of crystals on the femtosecond time scale (millionth of a billionth of a second) and phase transitions (melting and freezing) under extreme conditions, and to help detect dangerous materials remotely. These novel sources make practical use of two of Einstein's main ideas: special relativity and photons. The x-ray photons are produced by colliding relativistic electrons with an ultrashort, coherent laser pulse. The Doppler effect (analogous to the increasing pitch of an approaching police siren) dramatically shortens the wavelength of the incident light, from approximately 1 μm down to 0.1 Å. This poster will introduce the relevant physics concepts and the advanced technologies used in our research and highlight our progress and results.

The Wave/Particle Duality of Light

Richard Bionta

Einstein's 1905 work was the first use of light's wave/particle duality—the notion that light sometimes behaves as waves and sometimes behaves as particles—to explain the subtle particle behavior of visible light. Scientists at the time were confused because the long wavelengths of visible light overwhelmed its particle properties. In contrast, the wave properties of x rays are difficult to observe because of their short wavelengths, and the particle properties of x rays are dominant because of the large energy packed into each x-ray quantum.

The Linac Coherent Light Source (LCLS), now under construction at Stanford Linear Accelerator Center and scheduled to become operational in 2009, will be the world's first x-ray free electron laser, producing a coherent (wave-like) beam of intense x rays (10 trillion coherent photons) in 250-fs pulses for studies of short, fast interactions of light and matter and its movement (Brownian motion) on very short time scales. Since the LCLS produces a coherent x-ray beam, the wave properties are tremendously enhanced over conventional x-ray sources, allowing us to explore new states of



matter, follow chemical reactions and biological processes in real time, image materials on the nanoscale level, and image noncrystalline biological materials at atomic resolution.

Shining New Light on High-Energy Physics: Photon Colliders at the High-Energy Frontier

Jeff Gronberg

To the scientists of the 19th century, light was composed of amorphous electromagnetic waves that permeated space but could not interact with each other. The groundbreaking experiments of Einstein on the photoelectric effect turned this understanding on its head. With this understanding, a way to create photons of enormous energy was revealed: simply bounce light from a charged particle of high energy, like billiard balls colliding. Photon colliders can produce photons with energies only seen in nature in the explosions of supernovas. These high-energy photons can be a unique probe into elementary particle physics. When two photons collide, they can be converted into a charged-particle/antiparticle pair. Through the $E = mc^2$ formula, the entire energy of the photons is converted into the mass-energy of the particle/antiparticle pair, allowing particles that have not existed since the Big Bang to be produced.

Exploiting the Duality of Light in Photonic Integrated Circuits and Fiber-Based Systems

Tiziana Bond

The wave-particle dual nature of light is explored for complex signal processing, communication, and detection functionalities and achieved with both miniature-size integrated circuits on a chip and fiber-based systems on a bench. Photons generated in lasers are coupled and propagated as electromagnetic waves along optical waveguides, then manipulated to import external signal features or improve their spectral and time characteristics, to eventually be detected in forms of photons again through the photoelectric effect. This poster shows how we are putting photons to work, from the infrared to the ultraviolet, for all-optical switching by exploiting class III-V semiconductors and advanced etching techniques, from high-speed digital logic circuits, to highly sensitive radiation detectors and recorders at both the integrated and discrete levels.

X-Ray Tomography from High-Energy-Density Physics Targets to Michelangelo's David

Harry Martz

In one stroke, Einstein showed both that light is a stream of particles and also that there was solid evidence for the existence of waves. His theory could satisfactorily explain all the known

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properties of the photoelectric effect and was the first result derived from quantum theory of the interaction between radiation and matter. Light, i.e., the electromagnetic spectrum, behaves like a wave under certain conditions and like a stream of particles under others. In other words, it has a *dual nature*: we can understand it as either wave or particle, depending on our context of observation. We are taking advantage of the dual nature of x rays and their interaction with matter to conduct nondestructive characterization of various objects, from those as small as poppy seeds, through NASA space shuttle components, to Michelangelo's David.

Our study examines the refractive wave effects of x rays at low energies (a few keV) and high-spatial (~1-μm) resolution to characterize the deuterium–tritium ice-gas boundary layer in inertial-confinement-fusion targets. The photoelectric nature of x rays is useful to characterize high-energy-density physics targets in three dimensions. Medium energy (~100-keV) x rays are useful for characterizing NASA space shuttle components, and high-energy (~4-MeV) x rays can help inspect surface cracks in the ankles of Michelangelo's 500-year-old marble statue of David, which is located in the Galleria dell'Accademia museum in Florence. Assessing the volumetric extent of these cracks will provide information to the museum's art-conservation experts about how the cracks may affect the long-term structural stability of the statue.

The Solid-State Heat Capacity Laser

Bob Yamamoto

The Laboratory, under the sponsorship of the U.S. Army's Space Missile Defense Command (Huntsville, Alabama), has developed the world's most powerful solid-state (i.e. electric), diode-pumped laser called the solid-state heat capacity laser (SSHCL). The current laser system configuration has produced over 150 J/pulse at a pulse repetition rate of 200 Hz, equating to an average output power in excess of 30 kW. Because this laser produces significant amounts of power in a very small footprint, the military can use the laser as a directed-energy weapon in a variety of mobile configurations (land-, sea- and air-based). Potential target include rockets, artillery, and mortars; buried and exposed landmines; and improvised explosive devices (IEDs).

From the onset of the SSHCL program, LLNL has incorporated into their laser architecture several key enabling technologies supplied by industry. This was done to expedite the process of transforming a laboratory device into a hardened, battlefield-ready laser system. Present plans call for a 100-kW laboratory SSHCL to be

ready in 2007, with the potential for a megawatt-class SSHCL soon thereafter.

Janus Intense Short Pulse: The Next Ultrahigh Intensity Laser at LLNL
Andrew Ng

The Janus Intense Short Pulse (JISP) upgrade is being developed at LLNL to provide a high-energy (hundreds of joules), short duration (0.5 to 200-ps) laser pulse with variable delay from a second, high-energy (up to 1kJ), long-duration (0.2 to 20-ns) laser pulse on target. A new target chamber will allow the angle between the long and short pulse beams to be varied from about 35˚ to nearly 180˚, thus creating a unique Laboratory capability to support a wide range of experiments. For example, in the area of high-energy-density science, this new facility, called Janus II, will enable studies of dynamic material properties and equation of state under extreme conditions. In inertial confinement fusion, Janus II provides an experimental platform for fast ignition science. JISP is a significant tool in high-field-physics studies such as the production of antimatter (electron–positron) plasmas for exploring laboratory astrophysics. Commissioning of the system will begin in the summer of 2005.

Mapping Phonons at High-Pressure: Phase Transformation, Phase Stability, and Elastic Anisotropy
Dan Farber

This project represents LLNL's participation in an international collaboration to develop new techniques for mapping phonon dispersion curves (PDCs) at high pressure in the diamond anvil cell using high-resolution, inelastic x-ray scattering (HRIXS). The project will focus on probing PDCs in a number of physically novel systems: (1) Ce (an element often used as a surrogate for Pu) at or near the solid–solid singular point; (2) V at ultrahigh pressures; and (3) the high-pressure form (hexagonal closely packed) of Fe. If successful, this project will open a new field of research directed at probing the dynamics of systems at extreme conditions with HRIXS. Understanding the role of phonons in phase transitions is critical to our ability to describe the underlying physics that controls phase stability and a range of transport properties in lanthanide and actinide systems.

Ultrafast Science
Art J. Nelson

Ultrafast x-ray, electron beam and optical techniques combined with femtosecond lasers are powerful tools that can be used to probe the electronic and structural dynamics of molecules,

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biological systems, liquids, solids, surfaces, and interfaces as processes are occurring. Our work using these tools builds upon LLNL's research efforts in stockpile stewardship, which requires detailed knowledge of how materials respond to strong shocks and other extreme, nonequilibrium conditions. Experimental protocols, new physical concepts, and supporting theoretical tools are being developed to fully exploit the potential of such time-resolved techniques. LLNL has now embarked on a new strategic effort to develop time-resolved experimental capabilities that will position LLNL to become a worldleader in the advancement of science and methodologies in this new field.

Brownian Motion for Photons

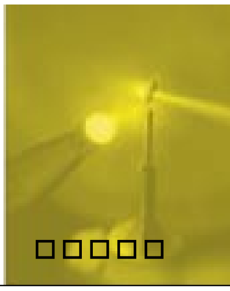
Bill Bateson

Brownian motion describes the trajectory of a test particle being knocked about by ambient particles. For the most part, the test particle moves in a straight line until random, impulsive collisions change its trajectory. The Einstein equations for radiation describe a similar process. Photons move in a straight line at a fixed speed. If the photon is absorbed by matter, then the matter shortly follows with spontaneous emission; thus the incident photon appears to have been scattered. This process of fixed-speed, straight-line motion with random scattering can be captured analytically.

Asymptotic Freedom in the Diffusive Regime of Neutron Transport

Britton Chang

The accuracy of a numerical method for solving the neutron transport equation is controlled by the smallest mean free path in the problem. Since problems in the asymptotic diffusive regime have vanishingly small mean free paths and computer memory is limited, solving these problems seems hopeless. However, we have found that the accuracy of a numerical method improves as the scattering



ratio increases with the mean free path and the grid spacing held fixed for problems in the asymptotic diffusive regime. This phenomenon is independent of the numerical method and can be explained on physical grounds. Accuracy improves as the scattering ratio increases because fewer neutrons are removed from the system. As a result, scattering frees the neutron distribution function from the rapid spatial variation, which is caused by absorption. Numerical results by the Diamond Difference Method are given to show this phenomenon.

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This research funded by Laboratory Directed Research and Development

From Stardust to Us: New Insight into Nuclear Synthesis from Heavy Stars, Supernova, Collapsars, and Gamma-Ray Bursts

Rob Hoffman

Most of the elements we encounter in everyday life were formed in the cores of massive stars, which end their lives in spectacular deaths heralded by a supernova explosion. These stars die because the conversion from mass to energy predicted by Einstein becomes inefficient as the star forms successively heavier elements. Ultimately the star collapses under its own gravity, a supernova is born, and newly formed heavy elements are expelled into the galaxy. These nuclear ashes eventually become our sun, our planet, and our bodies. We illustrate recent work on the synthesis of elements by stars that die in different ways and show that some elements—including zinc, copper and silver—may have their origins in stars so massive they collapse to form black holes. If so, the raw material for the pennies in our pockets is directly associated with the event horizons first predicted by Einstein's theory of gravity.

Perspectives on Gamma-Ray Bursts

Jay D. Salmonson

Gamma-ray bursts are touted to be the most powerful explosions in the known universe since the Big Bang. These distant, mysterious flashes of high-energy radiation have recently been discovered to be the last gasp in a fiery, explosive death of a distant star. But how and why such rare and powerful explosions take place is still unknown. This poster presents numerical simulations of possible gamma-ray-burst relativistic jet morphologies that address the question of the size and shape of the gamma-ray burst and its afterglow. By improving our understanding of what gamma-ray bursts look like, we will be better able to address the questions of how they work.

Characterization of Interplanetary Dust Particles by NanoSIMS and Transmission Electron Microscopy

Ian Hutcheon

Using nanoSIMS and transmission electron microscopy, we detected a 2175-Å absorption feature in 100-nm-size interstellar grains contained within carbon-rich interplanetary dust particles. The interstellar grains were identified on the basis of their nonsolar isotopic compositions. Although the 2175-Å extinction feature has been known as a spectral signature of dust in the interstellar medium for over 40 years, this discovery marks the first identification of actual carrier phases.

MACHO

Kem Cook

In the last decade, a number of projects have been mounted to detect and follow the progress of gravitational microlensing by compact objects, an extremely rare event. One of the original projects was the Massively Compact Halo Objects (MACHO) Project, a survey to determine whether the dark matter in the halo of the Milky Way has a significant baryonic component. The MACHO Project collected 8 years and 7.3 Tbyte of data on 99 square degrees toward the Magellanic Clouds and the bulge of the Milky Way. Half-square-degree fields were sampled, simultaneously in two bands, roughly every 3 days, and light curves for about 55 million stars to a depth of about magnitude 21 have been collected in a photometry database. This database has been analyzed for microlensing, and about 500 events toward the Bulge and about two dozen toward the Magellanic Clouds have been detected. Our analyses of these data have shown that microlensing has been detected, and all of the predicted variations due to the breakdown of the standard simplifying assumptions of point source, point lens, and uniform motion have been identified. Microlensing has been used to detect compact baryonic dark matter, to study stellar atmospheres at a level of detail impossible without microlensing, and to detect extra-solar planets.

Peering at the Origin of the Universe, Looking Deep without Blinking: LSST Survey of Dark Matter and Dark Energy.

Les Rosenberg

Based on Einstein's theoretical work, we know that the future of the Universe, whether it continues to expand forever or eventually contracts in a Big Crunch, depends on how much matter and energy it contains. The landmark observational work of Edwin Hubble in the 1920s profoundly changed our picture of cosmology by establishing that the Universe was indeed expanding. Two other discoveries in the 20th century contributed to the question of the fate of the Universe. Beginning in the 1930s, it became increasingly clear that galaxies, clusters of galaxies, and all large structures contained huge amounts of some new kind of matter, called "dark matter," which greatly outweighed the ordinary stuff of stars. Second, in the late 1990s, it was discovered that the expansion of the Universe is not slowing down but accelerating, implying the existence of a mysterious repulsive force, called "dark energy," whose energy density greatly exceeds even that of dark matter. We know neither what the dark matter or dark energy is. To illuminate these questions, LLNL is

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helping build the 8.4-m-diameter Large Synoptic Survey Telescope, which will look back in time at the distributions of dark matter and dark energy in the Universe. By looking for the subtle bending of light caused by dark matter, we can create a map of the distribution and evolution of dark matter going back billions of years. By carefully mapping out the red shift vs. distance for various objects, we can also map out the distribution of dark energy to enormous distances, and thereby constrain various theories for what dark energy might be.

Searching for Dark Matter Close to Home: Axion Dark Matter Experiment

Les Rosenberg

The amount of matter in the Universe has been of great interest to scientists since the time of Einstein. Dynamic observations of galaxies, clusters of galaxies and other large-scale structures in the Universe, as well as gravitational lensing, imply there are large amounts of dark matter in the Universe, i.e. stuff other than ordinary stars, planets, and gas clouds. We do not know what the dark matter is, but one prominent idea suggests that it is made up of one or more species of particle relics from the Big Bang. In the 1970s, Frank Wilczek, one of this year's Nobel Laureates, recognized that a minimal extension of the theory of the force that holds the atomic nucleus together predicts an additional elementary particle, the axion. The axion has all the properties to be an ideal dark matter candidate, i.e., it would be long-lived, possess vanishingly small interactions other than gravity, and be copiously produced during the Big Bang. For the past decade, a team led by LLNL has been looking for the axion by its resonant conversion to microwave photons in a cavity permeated by a strong magnetic field. This experiment already has a sensitivity sufficient to detect certain models of axions, should they exist. The experiment will soon become much more sensitive by incorporating new amplifiers, called SQUIDs, whose noise is approaching the irreducible limits of quantum mechanics.

Atomic X-Ray Spectra as a Probe of Black Holes

Duane Liedahl

Perhaps the most extraordinary result of Einstein's Theory of General Relativity is the prediction of black holes. Black holes, by definition, do not radiate electromagnetic energy. However, if a sufficient source of matter exists in the vicinity of a black hole—a nearby star, for example—then the gravitational field of the hole can capture this matter, creating a disk-

shaped configuration called an accretion disk. Matter gradually spirals inward through the disk, eventually reaching extreme relativistic velocities as it approaches the event horizon. The disk material heats up as it nears the event horizon, and becomes x-ray luminous. Spectroscopic measurements in the x-ray band thus provide probes of matter in the strong-field limit of gravitation.

Accreting black holes in binary systems, such as Cygnus X-1, constitute some of the brightest x-ray sources in the Galaxy. On a much larger scale, many galaxies, including our own, harbor black holes at their centers, with masses from millions to billions of solar masses, which accrete material from their local environments. Extreme examples of accretion onto supermassive black holes help to explain active galaxies and quasars, which emit thousands of times the total light of our Galaxy from a region comparable in size to our Solar System.

X-ray spectra from active galaxies obtained with the current generation of x-ray observatories reveal line emission that is modified by both special relativistic and general relativistic effects. It seems that we are witnessing matter orbiting in an accretion disk around a supermassive black hole as it prepares to cross the event horizon. Our project involves calculations of accretion disk structure, with the aim of elucidating the radiation processes near the event horizons of black holes.

High-Energy Astrophysics and Einstein

Michael Pivovaroff

The field of x-ray astronomy owes a huge debt to Albert Einstein. From explaining the physics behind the instrumentation, to providing the framework to interpret myriad observational results, his work has been crucial for explaining the way the Universe works. His explanation of the photoelectric effect (1905) is the mechanism used to generate x rays in the laboratory that are needed to calibrate high-energy detectors and telescopes. In 1918, he recognized that the index of refraction for x rays was less than unity—a fact that leads to the total external reflection of light, the basis of all focusing x-ray mirrors.

It wasn't until the late 1960s that technology allowed the development of the first x-ray telescopes, and it took another decade before NASA launched the first dedicated x-ray astronomy telescope, appropriately renamed *Einstein*. Over its 30-month mission, *Einstein* revolutionized our understanding of the x-ray universe. Since then, other x-ray telescopes, most recently the Chandra X-ray Observatory

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and XMM-Newton, have continued this advance. Einstein's theory of special relativity (1905) is needed to explain x-ray emission from a variety of systems, including how compact objects expel matter along their spin axes. These jets move at velocities close to the speed of light, and understanding their formation is an active area of research. Study of the interaction between the youngest neutron stars, referred to as pulsars, and their surrounding supernova remnants provide a unique opportunity to study a wide variety of phenomena.

Looking to the future, the field of x-ray astronomy will expand to higher energies, thanks to new technologies. LLNL has developed a new method for fabricating x-ray mirrors and will partner with several other institutions to launch NuSTAR, a path-breaking mission analogous to *Einstein* that will, for the first time, provide a detailed look into the x-ray universe above 10 keV.

The Creation of Neutron Star Atmospheres on NIF: A New Paradigm in Extreme Physics

Richard Klein

Einstein's 1905 paper on the quantification of light laid the foundation for further work on understanding radiation and its interplay with matter, further explored in his 1917 paper "On the Quantum Theory of Radiation." This paper fully characterized the particle-like properties of light. We use this theory to understand the physics present in extreme astrophysical environments such as those found in the polar atmosphere of a neutron star, where the radiation pressure can be larger than the particle pressure. Efforts are under way to develop a scaled experiment to reproduce these aspects in the laboratory, using NIF, the world's most powerful high energy laser, in tandem with the High Energy Petawatt laser when it becomes fully operational in several years. This research is leading the way to a new paradigm for studying the extreme physical conditions associated with compact astrophysical objects like neutron stars atmospheres and event horizons of black holes in an Earth-based laboratory.

Three-Dimensional Hydrodynamics Experiments on the National Ignition Facility

Brent Blue

The interaction of a shock wave with a density perturbation is a problem of basic scientific interest, with specific application to astrophysics and inertial confinement fusion (ICF). For instance, high-Mach-number

hydrodynamic jets, which can result from a shock/perturbation interaction, are ubiquitous features in astrophysics and may result from the presence of capsule joints or cryogenic fill tubes in ICF. Although the spatial scales of these systems vary over 16 orders of magnitude from supernovae jets (~10^{10} m) to micrometer-scale jets inside ICF capsules, they are unified by the physics of a high-Mach-number shock interacting with a perturbation at a two-fluid interface. The behavior of 2-D supersonic jets has previously been investigated in detail and compared to simulations over a wide range of conditions. In 3D, however, there are new aspects to the behavior of supersonic jets in compressible media. For example, a 3-D density perturbation that is at an angle to an incident shock is predicted to result in an asymmetric jet that evolves perpendicular to the incident shock in the compressible limit, and a tilted jet in the incompressible limit. This poster presents the NIF commissioning activities for hydrodynamics experiments as well as the results of the first set of hydrodynamics experiments on NIF.

Water under Extreme Conditions of Planetary Interiors.

Larry Fried

In a combined experimental and theoretical effort, we have determined the transition from molecular to nonmolecular water (the so-called superionic phase) under extreme pressures and temperatures like those found in planetary interiors. Raman spectroscopic experiments were performed in a laser-heated diamond anvil cell. The experiments found the loss of the OH stretch, indicative of a nonmolecular materials. The experimental phase boundary is in close agreement with theory, which indicates that the experimentally observed phase is a superionic (fast proton) conductor.

LLNL Envoy to the Planet Mercury

Monika Witte

The gamma-ray spectrometer (GRS), designed and built by a multilaboratory West Coast collaboration led by LLNL, is one of seven instruments aboard the NASA Messenger spacecraft on its mission to Mercury. The GRS will be used to help determine the abundance of elements in Mercury's crust. At the heart of the GRS is a germanium spectrometer that detects gamma rays coming from Mercury's surface. The germanium detector is made up of a germanium crystal that is cryogenically cooled and encapsulated in a gold-plated container with a nitrogen gas atmosphere. Because of its high-energy resolution, the GRS is sensitive enough to acquire very precise information from the planet's surface while it remains in space.

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In its most rudimentary form the GRS is a demonstration of Einstein's photoelectric effect: gamma rays of different energy levels from Mercury interact in the germanium, electron hole pairs are freed, and their motion creates image charge, thus forming the basis for the measurement of the energy levels in the elements on Mercury's crust. Because the detector needs to operate at a very cold temperature (approximately 87 K) while Messenger is so close to the Sun, the design or the thermal insulation to protect the detector was critical. Engineers from Lawrence Livermore and Lawrence Berkeley National Laboratories developed a design with three thermal shields and a cage held in place by Kevlar twine, thus supporting the detector during launch loads and providing thermal insulation during operation.

Slip-Rate Measurements on the Karakorum Fault in Tibet May Imply Secular Variations in Fault Motion

Rick Ryerson

Beryllium-10 surface exposure dating of offset moraines on one branch of the Karakorum Fault west of the Gar basin in Tibet yields a long-term (140- to 20-thousand-year) right-lateral slip rate of ~10.7 ± 0.7 mm per year. This rate is 10 times larger than that inferred from recent InSAR analyses (~1 ± 3 mm per year) that span ~8 years and sample all branches of the fault. The difference in slip-rate determinations suggests that large rate fluctuations may exist over centennial or millennial time scales. Such fluctuations would be consistent with mechanical coupling between the seismogenic, brittle-creep, and ductile shear sections of faults that reach deep into the crust. This somewhat controversial work is intimately tied to the analysis of information using global positioning systems that require active corrections for relativistic effects.

This research funded by Laboratory Directed Research and Development

Dynamic Data-Driven Event Reconstruction for Atmospheric Releases

Branko Kosovic

Atmospheric releases of hazardous materials have a rapid, high-consequence impact on large populations. For emergency response, sensor network design, and forensic needs, we are developing an event-reconstruction capability for use at the National Atmospheric Release Advisory Center. Our approach couples data and predictive models with Bayesian inference and stochastic sampling to provide backward analyses to determine unknown source characteristics, optimal forward predictions for consequence assessment, and dynamic reduction in uncertainty as additional data become available.

We use stochastic sampling methods to solve source inversion problems and compute source term parameters, taking into consideration measurement errors and forward model errors. Stochastic sampling methods are suitable even for the problems characterized by non-Gaussian distribution of source-term parameters. In this poster, we demonstrate our Markov Chain Monte Carlo (MCMC) event-reconstruction capability using data from the Prairie Grass and Copenhagen tracer field experiments. By using data from a subset of sensors and the operational Lagrangian particle dispersion code LOFI, the source location and source release rate can be identified. We have also developed and implemented a Stochastic Monte Carlo (SMC) capability to assimilate data dynamically as they become available.

How Does Atmospheric Turbulence Change in an Urban Environment?

Julie Lundquist

Due to their large populations, urban areas are particularly vulnerable to high-consequence accidental or intentional atmospheric releases of hazardous materials, and because of their complexity, urban environments present challenges for simulating atmospheric transport and dispersion.

To quantify the urban effect on atmospheric dispersion and to provide a dataset for the testing and validation of urban dispersion models, the Joint URBAN 2003 (JU2003) field experiment was funded by the Departments of Energy, Homeland Security, and Defense. LLNL, in collaboration with several other national laboratories and universities, mounted hundreds of meteorological and tracer instruments in and around the Oklahoma City urban core during July 2003. These instruments documented the evolving atmosphere and the effect of the Oklahoma City urban area on the state of the atmosphere. By releasing SF6, a passive tracer gas, in the city center, JU2003 groups

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(including a large LLNL contingent) explored the unique characteristics of dispersion in the urban area. Ongoing efforts in the Atmospheric Science Division are using these data for testing, validating, and improving the numerical models used in the National Atmospheric Release Advisory Center. This poster focuses on some unique aspects of urban meteorology revealed by the JU2003 experiment, particularly by the LLNL downwind profile.

Hindered Transport Phenomena in Complex Media

David Clague

The study of hindered transport phenomena involves the behavior of particles (e.g., colloids, macromolecules, and carrier particles) in complex media. Both convective processes—entrainment of particulate species with the suspending fluid—and diffusive processes govern particle rates of transport. In pure fluid, the entrained particles move with the velocity of the fluid and experience Brownian motion if they are at the colloidal scale. However, in a complex medium, like a physiological membrane, the suspended species experience hydrodynamic and colloidal interactions with the “fixed” surrounding medium, in this case the colloidal membrane, which contribute to hydrodynamic drag.

Starting in 1905, Einstein published a series of papers on Brownian motion and diffusion. From this body of work came the celebrated Stokes-Einstein equation for a Brownian sphere diffusing in a pure fluid. The equation derives from the balance of chemical potential and viscous resistance. However, in complex media, only the Stokes drag, not the viscous resistance, can be described. The drag must include hydrodynamic contributions from the fixed surrounding medium. Self-diffusive processes in complex media are said to be described by the generalized Einstein equation, which incorporates all of the hydrodynamic interactions experienced by diffusing particles. We use the generalized Einstein equation to describe diffusive processes in microfluidic devices, diffusion in polymers, and filtration processes relevant to Laboratory missions. Synergistically, the models and capabilities developed for Laboratory missions are directly applicable to describing and understanding diffusive processes at the physiological and cellular levels.

On the Movement of Small Particles in Liquids: Heat and Compression

Eric Schwegler

Recent advances in both experimental techniques and sophisticated theoretical methods have resulted in the discovery of fascinating new properties of materials under extreme conditions. In many instances, measurements alone are insufficient for a complete understanding of the emerging new phenomena. In such cases, ab initio methods have proven to be a useful complement for resolving ambiguities. First principles methods are also especially valuable for the prediction of properties where measurements do not yet exist. Our investigations on fluids are aimed at predicting and characerizing structural, electronic, and dynamical properties of materials under high temperature and pressure conditions by using a combination of different theoretical methods, including density functional theory, quantum Monte Carlo methods and quantum molecular dynamics.

Generalized Brownian Motion in Coarse-Grained Molecular Dynamics

Robb Rudd

Can Einstein's understanding of the random motion of pollen grains help us to resolve why cracks propagate at the wrong speed in computer simulations? It can, if we follow Einstein and focus on the unseen. In the computer simulation of materials, it is often desirable to direct computational power to the regions of the system where it is needed most. In finite element analysis, this motivation led to the development of adaptive mesh refinement; in atomistic simulation, the problem is more challenging, but the relatively recent development of concurrent multiscale simulation permits atomistic resolution of part of the system, coupled to a coarse-grained representation of other regions of the system. The coarse-grained model can be a conventional finite element model, and the resulting savings in computational expense permits the simulation of much larger systems. The invention of coarse-grained molecular dynamics (CGMD) made it possible to derive a generalized finite element formalism from the underlying atomistic dynamics directly for the first time. CGMD naturally recovers the atomistic force laws as the mesh is refined to the atomic scale. One result of this rigorous theory of concurrent multiscale coupling is that the coarse-grained modes are not deterministic; they experience random and dissipative forces due to the effective heat bath of the short wavelength modes that have been integrated out. Remarkably, this generalized Brownian motion resolves a long-standing issue with pathological energy flow when atomistic simulations are embedded in coarse-grained surroundings (including vacuum), best known from spurious wave reflections in fracture simulations that affect the crack propagation velocity. Thus, the

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action of the unseen degrees of freedom, just as in the motion of Brown's pollen grains, leads to unexpected and mystifying phenomena.

Quantum Simulation of High-Z Metals at Extreme Conditions

Randy Hood

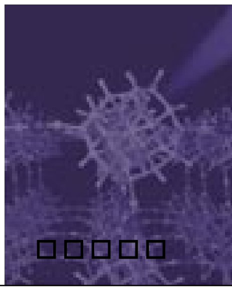
First-principles quantum simulations based on density-functional theory (DFT) have become a key area of research within the materials science, chemistry and condensed-matter physics communities. We have pioneered the development and use of these methods for high-*Z* metals with ground-breaking simulations of d- and f-electron materials on ASCI White, the Los Alamos National Laboratory's Q machine, and Thunder. We are now adapting our quantum molecular-dynamics (QMD) simulation code to meet the challenges of the revolutionary BlueGene/L (BG/L) machine, where new application horizons await, including materials aging and high-pressure melting. To harness the power of such large-scale computational platforms, it is critical to employ local methods to solve the DFT equations in order to minimize interprocessor communications. In the context of plane-wave-based QMD methods, substantial progress has already been made in this regard by localizing the required fast Fourier transforms (FFTs). Other real-space approaches such as the finite-element method are also being developed, and the successful adaptation of these to BG/L will provide tremendous new opportunities to study the properties of high-*Z* metals at extreme conditions. The poster presents available QMD simulation results from White, Q, Thunder and BG/L.

For more information, see http://www-phys.llnl.gov/Research/Metals_Alloys/index.html

Atomic-Scale Simulation of Rapid Resolidification in a Molten Metal on BlueGene/L

Fred Streitz

One-hundred years ago this month Albert Einstein published one of the seminal papers of the 20th century in which he described how Brownian motion, the apparently random motion of particles suspended in a liquid, arises from the thermal motion of atoms or molecules in a liquid. This paper is credited with ushering in a broader belief in the existence of atom and molecules, an issue that had been debated since antiquity. Although the acceptance of atoms is now taken for granted, we still seek to understand the apparently random motion of atoms in a liquid. Our investigative tool of choice is LLNL's BlueGene/L (BG/L), the largest computer in the world. With large-scale molecular dynamics, we



use BG/L to model the motion of hundreds of thousands of atoms in a liquid metal undergoing rapid compression to understand the process of solidification at extremes of pressure and temperature. Using advance quantum-based potentials to describe interatomic interactions and bond orientational order parameters to characterize the local structure, we demonstrate how the nucleation of a solid phase from the liquid is actually a gradual process stemming from countless random fluctuations in the liquid. A video sequence of the simulation demonstrates the stochastic nature of the event, one of the first successful scientific applications on BG/L.

First-Principles, Linear Scaling Electronic Structure Calculations

Jean-Luc Fattebert

Using modern computational methods, one can access molecular dimensions and even more complex details at the microscopic level, such as the nature of molecule–molecule interactions. We have devised and are implementing a new approach for accurate first-principles electronic structure calculations, whose complexity is proportional to the size of the system. This is a significant improvement over state-of-the-art methods, which generally scale as the cube of the number of atoms being simulated. The new method is based on localized electronic orbitals and real-space discretization, along with adaptive mesh refinement and multigrid methodologies to speed up computation. The superior scaling opens the door to solving problems that were previously considered intractable.

Concerning a Point of View on the Emission and Transformation of Light in Nanoparticles*

Andrew Williamson

Semiconductor nanoparticles are an exciting new class of materials with unique abilities to transform the properties of light. By controlling the size, shape, and composition of nanoparticles, their optical absorption and emission can be tuned from the infrared through to the ultraviolet, while maintaining high quantum efficiencies. These nanoparticles are already used in a range of nanotechnology applications, including biological imaging, telecommunications and solar cells. This poster presents the results of quantum mechanical simulations of the optical properties of silicon, germanium, carbon, and cadmium selenide nanoparticles. These simulations have been used both to interpret existing optical characterization experiments and to predict novel structures of nanoparticles with enhanced optical properties.

*Einstein's 1905 photoelectric effect paper is entitled "Concerning an heuristic point of view toward the emission and transformation of light."

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This research funded by Laboratory Directed Research and Development

Measurements of Protein Folding Kinetics Enabled by Fast Diffusive Mixing

Olgica Bakajin

Measurements of the kinetics of protein folding on the microsecond time scale are enabled by the development of microfluidic mixers, which allow us to access conformational changes of the protein under conditions far from equilibrium and at previously inaccessible time scales. The fastest mixing time we have reported is 8 µm, while reducing the sample consumption to femtomoles. In a single experiment, we can record time scales from under 10 µm to over 100 ms.

To achieve mixing on the microsecond time scale, we reduce the length over which the molecules need to diffuse by using hydrodynamic focusing. The equation that describes this diffusion was formulated by Einstein and explains how complex fluids, like the denaturant that prevents the protein from folding, diffuse into water. The equation was derived from the then still controversial idea of atoms and the observation that tiny pollen particles observed through a microscope can be seen to jiggle about (Brownian motion).

This poster describes the design and optimization of the mixers, using modeling of convective diffusion phenomena, and characterization of the mixer performance, using microparticle image velocimetry, dye quenching, and fluorescent resonance energy-transfer measurements of single-stranded DNA.

Physics of Biomineralization

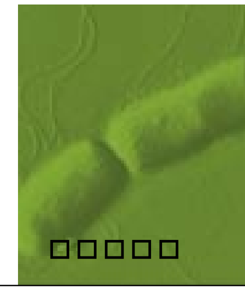
Chris Orme

Biological systems use peptides and proteins to direct the formation of mineralized tissue, thereby creating complex shapes and hierarchical composites not obtainable in the laboratory. Force microscopy is being used to understand the physical controls on biomineralization by directly imaging the growth of inorganic crystal surfaces in the presence of organic, peptide, and protein modifiers.

Big Physics in Small Spaces: Particle-Fluid Coupling in bioMEMS

David Trebotich

In 1827, British botanist Robert Brown noticed that pollen grains “jiggled” in water when observed under a microscope. He was never able to explain what caused this phenomenon. In 1905, unaware of previous observations, Albert Einstein showed that “according to the molecular-kinetic theory of heat, bodies of microscopically visible size suspended in



a liquid will perform movements of such a magnitude that they can be easily observed in a microscope, on account of the molecular motions of heat," and in doing so deduced the theoretical description of this so-called Brownian motion from statistical mechanics. Although his most famous formula, $E = mc^2$, comes out of his paper on relativity, his derivation of the diffusion relation in these papers has been the most significant for industry.

Today, we use Einstein's theoretical description of Brownian motion and diffusion to describe many phenomena in fluid dynamics. In biological flows, for example, the presence of large molecules in solution, coupled with the very small scales in state-of-the-art biochemical processors and sensors, brings about a new flow regime that is complex and not well understood. The coupling of fluid and particle dynamics is critical to high-fidelity models of these types of flows. At LLNL we have developed advanced numerical algorithms to model polymer-laden fluids in microfluidic devices. Based on a full coupling of particles and fluid we show that concepts derived in Einstein's seminal work—microscopic, Brownian motion and macro-scale, hydrodynamic viscous forces—play a role in manipulation of molecules in a microprocessor.

Measurement of Stoichiometries of Single Biomolecular Complexes using FRET Photon Statistics

Chris Hollars

We are using single-molecule spectroscopy combined with time-correlated single-photon counting (TCSPC) to make stoichiometric measurements of biolomolecular complexes. Using a TCSPC technique called photon antibunching, we determine the composition of the biomolecular complexes through the statistical analysis of the arrival of individual photons. The observation of this behavior is a benchmark for observing fluorescence from single molecules. We will apply this technique to the analysis of model systems followed by the analysis of protein DNA interactions.

Direct Determination of Affinity in Individual Protein–Protein Complexes in Mono- and Multivalent Configurations using Dynamic Force Spectroscopy

Todd Sulchek

Thermal energy causes rapid motions of biological macromolecules and their surrounding solvent. These molecular motions are known as Brownian motion, which Einstein helped explain in his 1905 paper. Brownian motion is

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responsible for the formation and breaking of all biological macromolecular bonds, which underpin all biological function. We have developed a method to directly measure these processes in a technique called dynamic force spectroscopy. We used the atomic force microscope to measure the binding forces between single molecule mucin1 (Muc1) protein and an antibody screened against Muc1. Muc1 is overexpressed on cell surfaces in a number of human cancers. Our collaborators at the UC Davis Cancer Center use antibodies to Muc1 as the targeting mechanism for delivery of radioimmunotherapeutic drugs, which consist of several such antibodies tethered to a common radioactive payload. Direct determination of binding affinities for mono- and multivalent configurations of such drugs is critical for their optimization. Such measurements depend on the ability to differentiate between mono- and multivalent bond formation. By measuring the binding strength as the function of the bond loading rate (dynamic force spectra), we determined energy barriers, thermodynamic off-rates, and the distance to the transition state for simultaneous dissociation of one, two, and three protein–protein pairs. This poster shows that although our measured bond strength scales linearly with the number of molecule pairs, the multivalent configuration leads to a precipitous decrease in the thermodynamic off-rates for the complex dissociation.

Understanding Protein–Small-Molecule Interactions using Computational Methods.

Felice Lightstone

Molecular recognition is the foundation of the interactions between a protein and small molecules. Using Newtonian and quantum physics, the atoms of the protein and small molecules can be modeled to predict their specific interactions. We have applied these algorithms to study different small molecules that interact and bind to the estrogen receptor, HLADR10, and tetanus toxin. Using computational methods, we are able to predict which class of molecules will bind to the surface of the proteins. With the proteins represented atomistically, molecular docking is used to predict where and how the small molecules bind the proteins. In collaboration with experimentalists, we have used these methods to help interpret experimental results, to design novel therapeutics, and to develop new reagents for biological assays.

The Mechanoelastic Properties of DNA Toroids

Larry Brewer

During spermiogenesis in mammals, histones in developing sperm chromatin are displaced coincident with the binding of the transition proteins, followed by the protamines, which condense and compact the genomic DNA into toroids. The toroids are further organized into a form that is extremely compact and transcriptionally inert, but whose higher order structure remains unknown. In an effort to understand how protamines and other sperm chromatin proteins contribute to this structure, we have constructed a dual optical trap with force-measuring capability to measure the elasticity of an individual DNA molecule as it is exposed to spermatid basic nuclear proteins in a novel microfluidic flow cell. We are interested in answering the following questions: (1) Do disulfide bonds form only between nearest neighbor protamine molecules bound along DNA, or can they form between any protamine molecules in close proximity to each other? In the latter case, we expect that disulfide bonds would lock adjacent loops of toroidal DNA together, making it impossible to extend the DNA molecule to its full contour length. (2) In the absence of disulfide bond formation, does protamine still stabilize DNA by binding in the major groove? We will see if the binding of protamine prevents the DNA B-to-S form ("overstretching") transition from occurring. The poster reports on the progress made on these experiments and the interpretations of the results, leading to better understanding of the higher order structure of sperm chromatin.

Nano-traincars Moving down DNA tracks: Single-Molecule FRET and Simulations of a DNA Sliding Clamp Moving along DNA.

Daniel Barsky

Like "nano-traincars" on tracks, DNA sliding clamp proteins can "ride" more than 10,000 bases along a DNA double helix (> 3 m linear distance). The clamps can also be driven by protein motors and can carry other proteins along. The clamps accomplish this by encircling the DNA, a unique topology in biology. In the absence of other proteins, DNA sliding clamps apparently slide freely along the DNA, yet analysis of the protein structures reveals many positive charges along the inner ring that should create strong salt bridges with the DNA. Why then do the clamps not remain stationary on

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the DNA? And how can clamps proceed past sizeable distortions in the DNA double helix? By a combined experimental and computational approach, we have investigated the interactions between DNA and a DNA sliding-clamp protein, the beta subunit of pol III. Our molecular dynamics simulations have illuminated the details of the DNA–protein interactions, and we are using single-molecule fluorescent resonant energy-transfer (FRET) measurements to infer the speed and diffusional character of the clamp's translocation.

Nuclear Physics

This research funded by Laboratory Directed Research and Development

Fusion and Fission: Converting Mass to Energy (or As Einstein Would Say: E = mc²)

Jeffery Latkowski

Einstein's famous equation, $E = mc^2$, indicates the equivalency of mass and energy. It is this relationship that lets us understand the power source of the Universe, thermonuclear fusion. It explains not just fusion, but also the basis of nuclear fission and fission power plants that already supply a significant fraction of electric energy (~20% in the US and more than 75% in France). In practice, we use Einstein's equation to determine the energy release from nuclear reactions by comparing the mass of the initial nuclei to the mass of the resultant nuclei. In the most common fusion reaction being studied around the world today, two isotopes of hydrogen, deuterium and tritium, fusion to form a helium nucleus (also known as an alpha particle) and a free neutron. The sum of the mass of the alpha and neutron is less then the sum of the mass of the deuterium (D) and tritium (T) by 0.019 atomic mass units (amu). This loss of mass results in a release of 17.6 MeV in the form of kinetic energy of the alpha and neutron. The conversion from mass to energy is at the rate of ~931 MeV/amu. Likewise, if we compare the mass of the fission products to the reactants, in this case a neutron and a fissile isotope of uranium or plutonium, we find a loss of nuclear mass and conversion to kinetic energy of the fission products, about 220 MeV per fission reaction. To appreciate the magnitude of the energy released in fusion and fission reactions following Einstein's law, consider that the burning of 1 kg of D and T in fusion reactions releases the same energy as burning ~10 million kg of coal, and the fission of 1 kg of uranium releases the equivalent of burning 12,000 barrels of oil. These nuclear reactions also have the benefit of not releasing any greenhouse gases, thus providing an attractive option for supplying the growing energy needs of our world.

Studies of Inertial Confinement Fusion Targets with HYDRA

Marty Marinak

This poster describes various physics issues important in inertial confinement fusion targets and shows examples of how these are modeled with the 3-D multiphysics code, HYDRA. Simulations performed on Livermore's massively parallel computers study the performance of ignition targets for the NIF. HYDRA can simulate the entire ignition target, including the hohlraum, capsule and all significant features. Simulations model intrinsic asymmetries that result from the ideal laser illumination pattern and those that result from effects of irregularities in laser pointing and power balance. High-resolution

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simulations study the evolution of hydrodynamic instabilities that occur when the capsule implodes. HYDRA calculates all of the radiation, electron, ion and charged-particle transport, and the hydrodynamics from first principles, i.e., no adjustments are made to the modeling parameters.

Prospects for Demonstrating Ignition on the National Ignition Facility in 2010 with Noncryogenic Double-Shell Targets

Peter Amendt

According to Einstein's mass–energy relationship, a nuclear reaction, which is exothermic, releases energy proportional to the mass difference between the initial and final nuclear states. We exploit this relationship to consider fusing deuterium and tritium into helium and a 14.1-MeV neutron with aid of the expected high-energy-density of the NIF laser in 2010. The double-shell ignition target design is one of several paths to demonstrating controlled thermonuclear ignition by potentially harnessing the energy of the 14.1 MeV neutrons that are liberated in the fusion reaction. A significant advantage of the double-shell target is the potential for fielding at room temperature, thereby avoiding the need for costly and challenging cryogenic preparation. This poster will highlight the advantages and challenges of demonstrating double-shell ignition on the NIF in 2010, while offering a balanced assessment of the prospects for success.

Exploring the Fast-Ignition Approach to Fusion Energy

Richard Town

Probably the most famous equation in physics is Einstein's $E = mc^2$, which was contained within his fifth and final paper published in 1905. The fusion process exploits this relationship between energy (E) and mass (m) to generate energy. When two isotopes of hydrogen [normally deuterium (D) and tritium (T)] fuse, they form an atom of helium and a neutron. In this process, some of the mass of the hydrogen is converted into energy. In the fast-ignition approach to fusion, a large driver (such as the NIF laser) is used to compress the DT fuel to extremely high densities, which is then "sparked" by a high-intensity, short-pulse laser. Understanding the transport of this short-pulse laser energy to the DT fuel is the critical issue explored in this poster.

Simulating the National Ignition Facility with Arbitrary Lagrangian Eulerian Methods and Adaptive Grids

Alice Koniges

Advanced 3-D computer simulations are enabling the design and operation of the NIF.

Experiments on NIF exemplify two of Einstein's 1905 ideas—the quantization of light allows production of a laser that will drive a fusion ($E = mc^2$) reaction. However, the reality of these regimes (in 2005 and beyond) produced by the high-energy facility requires state-of-the-art simulations to predict the effect of the laser-vaporized and -fragmented material on the target chamber. The poster discusses the use of arbitrary Lagrangian Eulerian (ALE) methods alone and ALE combined with adaptive mesh refinement to create a powerful simulation technique. LLNL's highly parallel computing facilities enable these compute-intensive calculations.

New Energy Sources: Extracting Energy from Radioisotope Materials

Jeff Morse

Are we tired of our cell-phone batteries dying while we're talking? These problems may be solved in the future by using nuclear-powered batteries that will exploit the energy stored in common radioisotope materials. Typically, this energy is emitted from radioisotopes as a range of energetic particles and photons. While many of these particles can be harmful to humans, a select group of radioisotopes are limited to particles called alphas, which are fairly benign and are readily absorbed over distances much less than the width of a human hair in most materials, including skin and clothes. We have embarked on a research effort to efficiently convert these energetic particles to useful electric power. Of the various energy conversion techniques, the poster reviews and presents results for thermal-to-electrical and direct alpha-voltaic energy-conversion approaches. Increasing the conversion efficiency for these approaches to levels by more than 20 % make them competitive with other power generation schemes at the microscale. So, while it may be years before we receive regulatory permission to use these power sources in consumer products, it is likely that they will be introduced for applications such as remote sensors and communications networks.

Production of Superheavy Elements

Ken Moody and Josh Patin

The search for superheavy elements explores the reaches of the Periodic Table and wouldn't be possible without a fundamental understanding of Einstein's work on inertia, energy, and special relativity. The production and separation of the heaviest elements is performed through the use of large particle accelerators and small-scale physical separation techniques. Understanding how particles interact when accelerated at one another and how matter is turned into energy

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is important to the design of the experiments that have successfully discovered several new elements of the Periodic Table. Understanding Einstein's special relativity has helped determine the chemistry of these heaviest elements and their place in the Periodic Table.

Nuclear Physics from Scratch: Ab-initio Description of Nuclei with Effective Interaction

Eric Ormand

How much does the nucleus weigh? Not surprisingly, the nucleus, consisting of protons and neutrons, weighs less than the sum of the mass of its constituents. This is due to the fact that protons and neutrons interact with one another via the strong interaction, and as a consequence are bound together. The energy required to bind this system of individual particles together, called the binding energy, reduces the total mass of the nucleus. This is a direct consequence of the Einstein mass–energy equivalence relation, $E = mc^2$. Perhaps the most important impact of nuclear binding is that some of this binding energy can be released in nuclear reactions, both fusion and fission.

After 50 years of intense study, the conceptually simple task of "building" complex nuclei from their constituent parts—protons and neutrons—has yet to be fully realized. The nucleus is a rich, complex quantum system whose constituents interact in ways that are extraordinarily complex, and not yet fully understood. Here at LLNL, the Nuclear Theory and Modeling Group is pursuing this topic with the goal of achieving a fundamental understanding of these complex phenomena from a unified theoretical standpoint. Our primary goal is to theoretically "build" nuclei from their constituents and the fundamental interactions between them, thus deriving nuclear structure from "scratch."

Finding Fission with Scintillator and a Stopwatch: Statistical Theory of Fission Chains

Neal Snyderman

Detailed information about fissioning materials can be extracted from the time of arrival of neutron and gamma ray counts. Analysis of the timing signal is based on a little-known theory first proposed by Feynman during the Manhattan project.

There are different numbers of neutrons and gamma rays emitted in each fission. Each of the created neutrons can induce a subsequent fission with some probability, establishing a chain of fissions that creates many neutrons and gamma rays starting from one neutron. The multiplication process amplifies the intrinsic fluctuations in the number of emitted particles from each induced fission. Any random emission process leads to a series of counts in a detector

in time that is a special probability distribution, a Poisson distribution. Complete randomness is very special, arising fundamentally from the complete randomness of quantum mechanics. The large fluctuations in the number of neutrons and gamma rays emitted in time from fission chains creates a pattern of counts in time that stands out sharply relative to this random distribution.

Mass to Energy: How Einstein's Equation is Helping Homeland Security

Jason Pruet

Finding fissile material hidden in sea-going cargo containers is a major security challenge issue around the world security and presents a real challenge because cargo containers are large and carry nearly every material found in modern commerce. However, recent experiments and calculations at LLNL indicate that the solution may be found in observing the conversion of mass to energy first predicted by Einstein's equations. This poster presents recent work on cargo interrogation techniques that rely on observing the energy released as heavy nuclei are ripped apart.

Nuclear Car Wash

Dennis Slaughter

A weak neutron beam is used to produce fission in special nuclear material that may be hidden in cargo. The subsequent delayed radiation produced by decaying fission products is very intense and distinct from background radiation so that even small quantities of illicit material can be detected. The beam is weak enough so that the cargo is not damaged and the dose to operating personnel or stowaways is well within government guidelines.